

=> file registry  
FILE 'REGISTRY' ENTERED AT 16:32:07 ON 20 JUL 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUL 2006 HIGHEST RN 894691-89-5  
DICTIONARY FILE UPDATES: 19 JUL 2006 HIGHEST RN 894691-89-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> file hcaplus  
FILE 'HCAPLUS' ENTERED AT 16:32:10 ON 20 JUL 2006  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2006 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

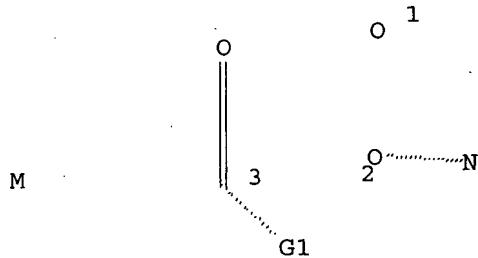
FILE COVERS 1907 - 20 Jul 2006 VOL 145 ISS 4  
FILE LAST UPDATED: 19 Jul 2006 (20060719/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.  
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

```
=> d stat que L74
L40    2034666 SEA FILE=REGISTRY ABB=ON   PLU=ON   T1/PG
L41    980214  SEA FILE=REGISTRY ABB=ON   PLU=ON   T2/PG
L42    604750  SEA FILE=REGISTRY ABB=ON   PLU=ON   T3/PG
L43    2951684 SEA FILE=REGISTRY ABB=ON   PLU=ON   (L40 OR L41 OR L42)
L47          STR
```

G2



G1 [@1], [@2]

G2 [@3], [@4]

Structure attributes must be viewed using STN Express query preparation.

```

L49      720204 SEA FILE=REGISTRY ABB=ON PLU=ON L43 AND N>2
L51      92776 SEA FILE=REGISTRY SUB=L49 SSS FUL L47
L52      64415 SEA FILE=HCAPLUS ABB=ON PLU=ON L51
L53      63198 SEA FILE=HCAPLUS ABB=ON PLU=ON "MASS SPECTROMETRY"/CW
L56      145097 SEA FILE=HCAPLUS ABB=ON PLU=ON TRANSITION METAL?/OBI
L62      129778 SEA FILE=HCAPLUS ABB=ON PLU=ON MASS SPECTROM?/OBI
L63      229730 SEA FILE=HCAPLUS ABB=ON PLU=ON MASS SPECTROM?/BI
L66      179531 SEA FILE=HCAPLUS ABB=ON PLU=ON TRANSITION METAL?/BI
L72      705 SEA FILE=HCAPLUS ABB=ON PLU=ON L52 AND (L53 OR (L62 OR L63))

L73      QUE ABB=ON PLU=ON ?PEPTID?/BI
L74      9 SEA FILE=HCAPLUS ABB=ON PLU=ON L73 AND L72 AND (L56 OR L66)

```

=> d ibib abs hitind hitstr L74 1-9

L74 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2006:564739 HCAPLUS  
 DOCUMENT NUMBER: 145:58819  
 TITLE: Labeled transition metal complexes  
       for labeling chemical or biological entities for  
       mass spectrometry  
 INVENTOR(S): Lacombe, Marie; Opdam, Franciscus Johannes Marie;  
               Talman, Eduard Gerhard; Veuskens, Jacky Theo Maria  
 PATENT ASSIGNEE(S): Kreatech Biotechnology B.V., Neth.  
 SOURCE: PCT Int. Appl., 91 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent

LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE     |
|---|------|----------|-----------------|----------|
| WO 2006062391   | A1   | 20060615 | WO 2005-NL824   | 20051201 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW |      |          |                 |          |
| RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  |      |          |                 |          |
| EP 1669760  | A1   | 20060614 | EP 2004-78328   | 20041208 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU   |      |          |                 |          |

PRIORITY APPLN. INFO.: EP 2004-78328 A 20041208  
 AB The invention relates to a labeled **transition metal** complex comprising a **transition metal** atom, a reactive moiety for allowing a chemical or biol. entity to become attached to the **transition metal** atom, an inert tridentate moiety as a stabilizing bridge, and a marker. The invention also relates to a labeled chemical or biol. entity comprising a chemical or biol. entity which is attached

to said labeled **transition metal** complex, to the use of said complex for creating a defined shift in the mol. mass of said entity in order to facilitate **mass spectrometric** anal. of said entity, to methods for rendering chemical or biol. entities distinguishable by **mass spectrometry** as well as to methods for **mass spectrometric** anal. of the chemical or biol. entities. In addition, the present invention also relates to a set of at least two of said **transition metal** complexes of different mol. mass, to **transition metal** complexes comprising different stable isotopes, to chemical or biol. entities obtained by a method of the invention and to a kit of parts supporting the use and/or methods of the invention. 4'-Aminopentyl ether-2,2':6',2"-terpyridine (APET), prepared from 5-aminopentanol and 4'-chloro-2,2':6',2"-terpyridine, was coupled with EZ-link-LC-biotin succinimidyl ester and complexed with K2PtCl4. The complex was used to label proteins and DNA.

CC 9-5 (Biochemical Methods)

Section cross-reference(s): 28, 29, 78

ST labeled **transition metal** complex labeling **mass spectrometry**; biotin aminopentyl ether terpyridine platinum complex labeling protein; DNA labeling biotin aminopentyl ether terpyridine platinum complex

IT Nucleic acid hybridization

(DNA-DNA, in situ; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Antibodies and Immunoglobulins

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (IgA, labeling of; labeled **transition metal**)

complexes for labeling chemical or biol. entities for mass spectrometry)

IT Antibodies and Immunoglobulins  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(IgG; labeling of; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Antibodies and Immunoglobulins  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(IgM, labeling of; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Ionic strength  
(agents for adjustment of; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Glycosides  
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(amino, aminoglycosides, labeled with labeled transition metal complex; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Samples  
(anal. of; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Phosphate group  
(as reactive group in labeled transition metal complex; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Bicarbonates  
Bromides, reactions  
Carbonates, reactions  
Chlorides, reactions  
Fluorides, reactions  
Iodides, reactions  
Nitrates, reactions  
Phosphonates  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(as reactive group in labeled transition metal complex; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Immunoassay  
(enzyme-linked immunosorbent assay; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Immunoassay  
(immunoblotting; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Fluorescent substances  
(in labeled transition metal complex; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT Buffers  
Human

**Mass spectrometry**  
Microarray technology  
**Tandem mass spectrometry**  
Test kits  
Test tubes  
(labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT Polyoxyalkylenes, reactions  
Transition metals, reactions  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT Amines, biological studies  
Amino acids, biological studies  
Enzymes, biological studies  
Glycoproteins  
Nucleosides, biological studies  
**Oligopeptides**  
Peptide nucleic acids  
Phospholipids, biological studies  
Polynucleotides  
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic  
preparation); BIOL (Biological study); PREP (Preparation)  
(labeled with labeled transition metal complex;  
labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT Antibodies and Immunoglobulins  
Nucleic acids  
Nucleotides, biological studies  
Oligonucleotides  
**Peptides**, biological studies  
Proteins  
RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic  
preparation); BIOL (Biological study); PREP (Preparation)  
(labeled, with labeled transition metal complex;  
labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT **Transition metal complexes**  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(labeled; labeled transition metal complexes for  
labeling chemical or biol. entities for mass  
spectrometry)

IT Plasmids  
(labeling DNA of; labeled transition metal  
complexes for labeling chemical or biol. entities for mass  
spectrometry)

IT Biochemical compounds  
Chemical compounds  
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
(labeling and mass spectrometry of; labeled  
transition metal complexes for labeling chemical or  
biol. entities for mass spectrometry)

IT HeLa cell  
(labeling lysate proteins of; labeled transition  
metal complexes for labeling chemical or biol. entities for  
mass spectrometry)

IT DNA  
Proteins  
RNA

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (labeling of; labeled **transition metal** complexes  
 for labeling chemical or biol. entities for **mass spectrometry**)

IT Mass  
 (solar; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Isotopes  
 RL: PRP (Properties)  
 (of **transition metal**, complexes containing; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Carboxylic acids, reactions  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (salts, as reactive group in labeled **transition metal** complex; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Functional groups  
 (sulfate, as reactive group in labeled **transition metal** complex; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Enzymes, biological studies  
 RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (synthetic, labeled with labeled **transition metal** complex; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT Analytical apparatus  
 (test strips; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 146368-14-1D, Cy5, conjugate with APET, platinum and ruthenium  
 146368-16-3D, Cy3, conjugate with APET-Pt 890935-62-3D,  
 conjugate with Cy5 890935-70-3D, conjugate with Cy3 and Cy5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (DNA labeling with; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 64-19-7, Acetic acid, reactions 71-50-1, Acetate, reactions 77-92-9,  
 reactions 126-44-3, Citrate, reactions 144-62-7, Ethanedioic acid,  
 reactions 338-70-5, reactions 625-58-1, Ethylnitrate 7732-18-5,  
 Water, reactions  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (as reactive group in labeled **transition metal** complex; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 111-40-0, Diethylenetriamine  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (complexation of; labeled **transition metal** complexes for labeling chemical or biol. entities for **mass spectrometry**)

IT 890935-60-1 890935-61-2  
 RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent); USES (Uses)

(labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 890935-50-9P  
 RL: ARG (Analytical reagent use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 890935-52-1 890935-53-2 890935-54-3 890935-55-4 890935-56-5  
 890935-57-6 890935-58-7 890935-59-8  
 RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)  
 (labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 890935-49-6P  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 79-04-9, Chloroacetyl chloride 107-13-1, Acrylonitrile, reactions  
 107-14-2, Chloroacetonitrile 107-15-3, Ethylenediamine, reactions  
 627-42-9, 2-Chloroethyl methyl ether 1001-53-2, N-Acetylenediamine  
 2508-29-4, 5-Aminopentanol 7439-88-5D, Iridium, complexes 7439-89-6D,  
 Iron, complexes 7439-96-5D, Manganese, complexes 7439-98-7D,  
 Molybdenum, complexes 7440-02-0D, Nickel, complexes 7440-04-2D,  
 Osmium, complexes 7440-05-3D, Palladium, complexes 7440-06-4D,  
 Platinum, complexes 7440-16-6D, Rhodium, complexes 7440-18-8D,  
 Ruthenium, complexes 7440-33-7D, Tungsten, complexes 7440-43-9D,  
 Cadmium, complexes 7440-47-3D, Chromium, complexes 7440-48-4D, Cobalt,  
 complexes 7440-50-8D, Copper, complexes 7440-62-2D, Vanadium,  
 complexes 7440-66-6D, Zinc, complexes 10025-99-7 25322-68-3,  
 Polyethylene glycol 51857-17-1 62572-85-4 72040-63-2 92557-81-8  
 128143-89-5 139346-57-9 150810-69-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 111-40-0DP, Diethylenetriamine, complex with platinum compds.  
 86240-79-1P 194213-77-9P 201282-04-4P 672304-28-8P 869484-26-4P  
 890648-50-7P 890648-51-8P 890648-55-2P 890648-56-3P 890648-57-4P  
 890648-58-5P 890648-59-6P 890648-60-9P 890648-61-0P 890935-47-4P  
 890935-48-5P 890935-65-6P 890935-66-7P 890935-68-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 890648-52-9P 890648-53-0P 890648-54-1P 890935-69-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

IT 75909-25-0  
 RL: BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)  
 (labeling of; labeled transition metal complexes  
for labeling chemical or biol. entities for mass  
spectrometry)

IT 890935-63-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and HeLa cell lysate protein labeling with; labeled  
transition metal complexes for labeling chemical or

biol. entities for mass spectrometry)

IT 890935-64-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and plasmid DNA labeling with; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT 890935-67-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation and protein labeling with; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

IT 890935-51-0

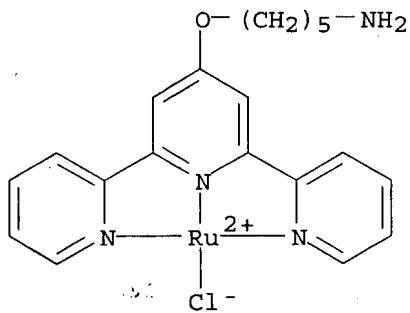
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction with DNA; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

JT 890935-62-3D, conjugate with Cy5 890935-70-3D, conjugate with Cy3 and Cy5

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (DNA labeling with; labeled transition metal complexes for labeling chemical or biol. entities for mass spectrometry)

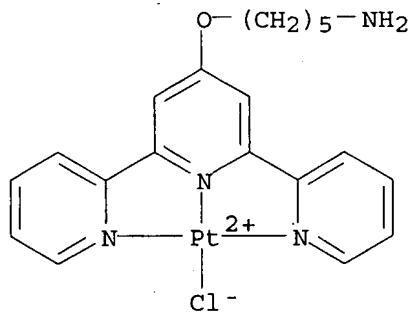
RN 890935-62-3 HCPLUS

CN INDEX NAME NOT YET ASSIGNED



RN 890935-70-3 HCPLUS

CN INDEX NAME NOT YET ASSIGNED

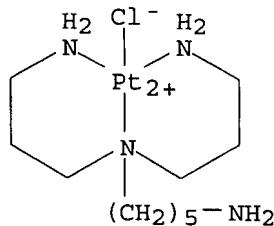


IT 890935-48-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(labeled transition metal complexes for labeling  
chemical or biol. entities for mass spectrometry)

RN 890935-48-5 HCAPLUS  
CN INDEX NAME NOT YET ASSIGNED



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L74 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:1354663 HCAPLUS

DOCUMENT NUMBER: 144:83644

TITLE: Methods for target molecule detection using siderophores and related compositions

INVENTOR(S): Bosse, Roger; Patton, Wayne F.; Roby, Philippe

PATENT ASSIGNEE(S): PerkinElmer Las, Inc., USA

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO.  | KIND | DATE     | APPLICATION NO. | DATE       |
|---|------|----------|-----------------|------------|
| WO 2005123954   | A2   | 20051229 | WO 2005-US20152 | 20050609   |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,<br>CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,<br>GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,<br>LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,<br>NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,<br>SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,<br>ZA, ZM, ZW |      |          |                 |            |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,<br>AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,<br>EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,<br>RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,<br>MR, NE, SN, TD, TG  |      |          |                 |            |
| US 2006019279   | A1   | 20060126 | US 2005-148478  | 20050609   |
| PRIORITY APPLN. INFO.:  |      |          | US 2004-521644P | P 20040609 |
|   |      |          | US 2004-521956P | P 20040727 |

AB The invention provides methods for isolating a target mol. from a sample. In an embodiment, the method involves contacting a sample with a capture agent, the agent comprising a siderophore and a transition metal cation, under conditions wherein the agent is capable of binding a target mol. to form a target mol.-capture agent complex, wherein the target mol. is selected from the group consisting of a phosphorylated

mol., a nitrotyrosine-containing mol. and a sulfated mol., and separating the target mol.-capture agent complex from the sample, thereby isolating the target mol. from the sample. Also provided are methods for determining the presence of a target mol. in a sample, that involve contacting a sample with a capture agent, the agent comprising a siderophore and a transition metal cation.

IC ICM C12Q001-68

CC 9-15 (Biochemical Methods)

IT **Peptides, uses**

RL: NUU (Other use, unclassified); USES (Uses)

(Amphibactins; methods for target mol. detection using siderophores and related compns.)

IT **Peptides, uses**

RL: NUU (Other use, unclassified); USES (Uses)

(Aquachelins; methods for target mol. detection using siderophores and related compns.)

IT **Peptides, uses**

RL: NUU (Other use, unclassified); USES (Uses)

(Marinobactins; methods for target mol. detection using siderophores and related compns.)

IT **Peptides, uses**

RL: NUU (Other use, unclassified); USES (Uses)

(exochelins; methods for target mol. detection using siderophores and related compns.)

IT **Transition metals, reactions**

RL: RCT (Reactant); RACT (Reactant or reagent)

(ions; methods for target mol. detection using siderophores and related compns.)

IT **Absorption**

Atomic spectrometry

Capillary tubes

Composition

ESR (electron spin resonance)

Ellipsometry

Filters

Gels

Mass

**Mass spectrometry**

Matrix media

Membranes, nonbiological

Microarray technology

NMR (nuclear magnetic resonance)

Particles

Phosphorylation, biological

Polarized fluorescence

Refractive index

Resonance fluorescence

SERS (Raman scattering)

Surface

Surface plasmon resonance

Transmissions (mechanical)

(methods for target mol. detection using siderophores and related compns.)

IT **Peptides, uses**

RL: NUU (Other use, unclassified); USES (Uses)

(methods for target mol. detection using siderophores and related compns.)

IT **Peptides, uses**

RL: NUU (Other use, unclassified); USES (Uses)

(ornibactins; methods for target mol. detection using siderophores and related compns.)

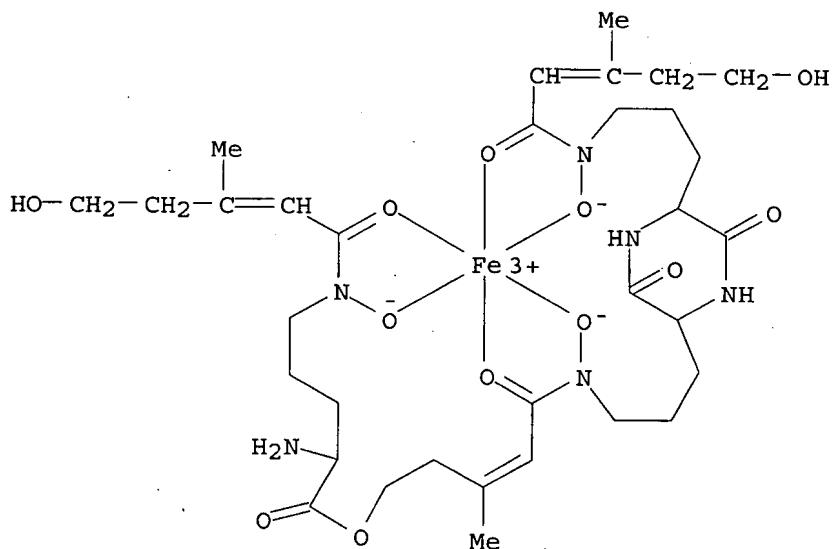
IT **Mass spectrometry**  
 (plasma-source, inductively-coupled; methods for target mol. detection using siderophores and related compns.)

IT 51-28-5, 2,4-Dinitrophenol, uses 58-85-5, Biotin 94-75-7, 2,4-Dichlorophenoxyacetic acid, uses 533-48-2, Desthiobiotin 1400-46-0, Mycobactin 1672-46-4, Digoxigenin 2396-01-2, Phenyl 8062-00-8, Pyoverdin 9001-45-0 9003-99-0, Peroxidase 9031-11-2,  $\beta$ -Galactosidase 11115-85-8, Fusarinine 12705-44-1, Coprogen B 12705-44-1D, Coprogen B, derivs. 15646-46-5 15788-16-6, 5-Benzimidazolecarboxylic acid 18928-00-2, Rhodotorulic acid 23086-46-6, Ferricrocin 23425-25-4, Ferrirubin 26912-16-3D, Dimerum acid, derivs. 28384-96-5, Enterobactin 35418-52-1, Schizokinen 72731-33-0, Cepabactin 79236-62-7 104022-79-9, Pyoverdin Pa A 114844-84-7, Azotobactin 120124-51-8, Chrysobactin 124620-50-4, EKD 3-88 131688-65-8, Azoverdin 134782-23-3, JAM-2-263 139917-13-8, Pseudobactin B 10 156737-07-4, Acinetoferrin 159074-16-5, Alcaligin E 197846-90-5, Pyoverdin G4R 207130-71-0D, Vicibactin, derivs. 214491-43-7, 6,8-Difluoro-4-methylumbelliferyl phosphate 344549-58-0 353512-65-9, Triacetyl fusarinine  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (methods for target mol. detection using siderophores and related compns.)

IT 12705-44-1, Coprogen B 12705-44-1D, Coprogen B, derivs.  
 RL: NUU (Other use, unclassified); USES (Uses)  
 (methods for target mol. detection using siderophores and related compns.)

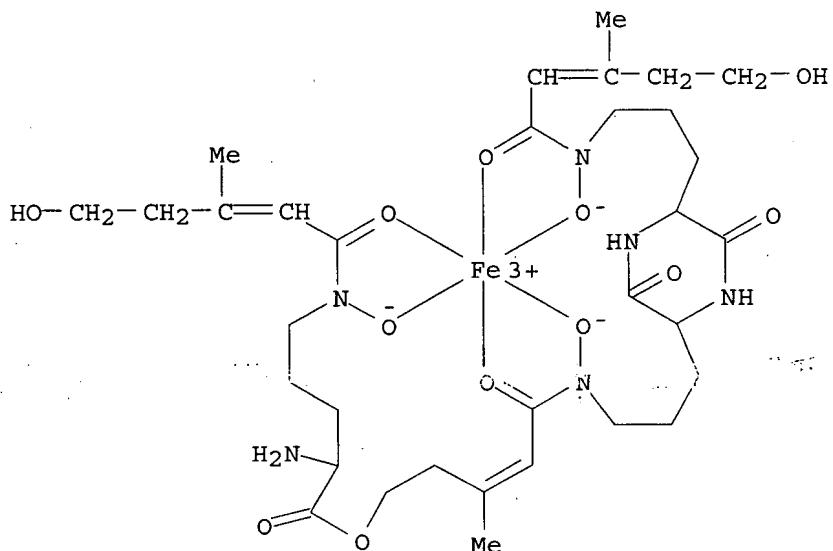
RN 12705-44-1 HCAPLUS

CN Iron, [5-[(hydroxy- $\kappa$ O) [3-[5-[(3-[(hydroxy- $\kappa$ O) [5-hydroxy-3-methyl-1-(oxo- $\kappa$ O)-2-pentenyl]amino]propyl]-3,6-dioxo-2-piperazinyl]propyl]amino]-3-methyl-5-(oxo- $\kappa$ O)-3-pentenyl N5-(hydroxy- $\kappa$ O)-N5-[5-hydroxy-3-methyl-1-(oxo- $\kappa$ O)-2-pentenyl]-L-ornithinato(3-)]- (9CI) (CA INDEX NAME)



RN 12705-44-1 HCAPLUS  
 CN Iron, [5-[(hydroxy- $\kappa$ O) [3-[5-[(3-[(hydroxy- $\kappa$ O) [5-hydroxy-3-

methyl-1-(oxo- $\kappa$ O)-2-pentenyl]amino]propyl]-3,6-dioxo-2-piperazinyl]propyl]amino]-3-methyl-5-(oxo- $\kappa$ O)-3-pentenyl  
N5-(hydroxy- $\kappa$ O)-N5-[5-hydroxy-3-methyl-1-(oxo- $\kappa$ O)-2-pentenyl]-L-ornithinato(3-)]- (9CI) (CA INDEX NAME)



L74 ANSWER 3 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:1028896 HCPLUS  
 DOCUMENT NUMBER: 143:471915  
 TITLE: Pyridine-Substituted Oligopeptides as Scaffolds for the Assembly of Multimetallic Complexes: Variation of Chain Length  
 AUTHOR(S): Ohr, Kristi; Gilmartin, Brian P.; Williams, Mary Elizabeth  
 CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA  
 SOURCE: Inorganic Chemistry (2005), 44(22), 7876-7885  
 CODEN: INOCAJ; ISSN: 0020-1669  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB This paper presents the synthesis and characterization of pyridine-substituted artificial oligopeptides with an aminoethylglycine backbone of varying length, which are designed to act as scaffolds for the self-assembly of multimetallic structures. The identities and purities of the oligopeptides are confirmed with mass spectrometry, <sup>1</sup>H NMR, HPLC, and pH titrns. The acid dissociation consts. for the oligopeptides were determined and were found to decrease with increasing pyridine units. Titrns. of the oligopeptides with Cu(II) and Pt(II) complexes containing the tridentate ligands 2,2':6',2''-terpyridine and pyridine 2,6-dicarboxylic acid were monitored using UV-visible absorption spectroscopy and showed stoichiometric binding based on the number of pyridines on the peptide strand. Metal titrns. performed using an analogous oligopeptide with Me substituents (in place of the pyridine ligands) showed very weak or no binding. In the case of the oligopeptides containing bound Pt(terpyridine)<sup>2+</sup> complexes, cyclic

voltammetry reveals two sequential 1-electron redns. at formal potentials that do not vary as a function of oligopeptide length. The measured diffusion coeffs. were measured with chronoamperometry and were found to decrease with increasing oligopeptide length.

CC 78-7 (Inorganic Chemicals and Reactions)  
 Section cross-reference(s): 34, 68, 72

ST oligopeptide pyridyl prepn acidity coordination  
 transition metal chelate; copper complex pyridyl  
 oligopeptide scaffold prepn; platinum complex pyridyl  
 oligopeptide scaffold prepn electrochem redox

IT Ionization constant  
 (acidity constant; of pyridine-substituted oligopeptides)

IT Redox reaction  
 (electrochem.; of pyridine-substituted oligopeptide scaffolds coordinated with copper(II) or platinum(II) chelates)

IT Chemical chains  
 (length; preparation of pyridine-substituted oligopeptide scaffolds, acid dissociation consts., and coordination with copper(II) or platinum(II) chelates)

IT Formal potential  
 Reduction potential  
 Self-assembly  
 (of pyridine-substituted oligopeptide scaffolds coordinated with copper(II) or platinum(II) chelates)

IT **Oligopeptides**  
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pyridine-substituted oligopeptide scaffolds, acid dissociation consts., and coordination with copper(II) or platinum(II) chelates)

IT 169396-89-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (N-acylation for preparation of pyridine-substituted oligopeptide scaffolds coordinated with metal(II) chelates)

IT 869190-58-9 869190-60-3 869190-62-5  
 869190-64-7 869289-03-2  
 RL: PRP (Properties)  
 (energy-minimized mol. structure from mol. mechanics calcns.)

IT 6622-91-9, 4-Pyridylacetic acid hydrochloride  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of pyridine-substituted oligopeptide scaffolds coordinated with metal(II) chelates)

IT 869190-67-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (for preparation of pyridine-substituted oligopeptide scaffolds coordinated with metal(II) chelates)

IT 220802-14-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (for preparation of tetramer oligopeptide scaffold)

IT 861886-02-4P 861886-04-6P 869190-49-8P  
 869190-50-1P 869190-51-2P 869190-53-4P  
 869190-55-6P 869190-57-8P 869287-59-2P 869288-33-5P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pyridine-substituted oligopeptide scaffolds coordinated with metal(II) chelates)

IT 869190-59-0P 869190-61-4P 869190-63-6P  
 869190-65-8P 869289-23-6P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (preparation, cyclic voltammetry, and diffusion coefficient measured with chronoamperometry)

IT 869190-59-9 869190-60-3 869190-60-7

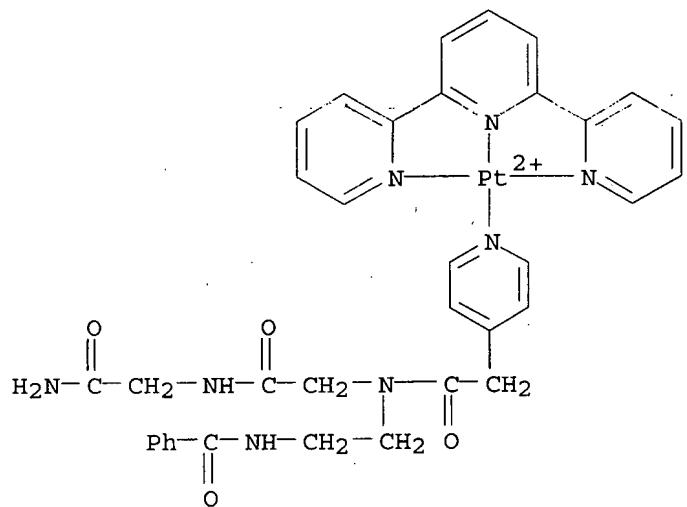
**869190-64-7**

RL: PRP (Properties)

(energy-minimized mol. structure from mol. mechanics calcns.)

RN 869190-58-9 HCPLUS

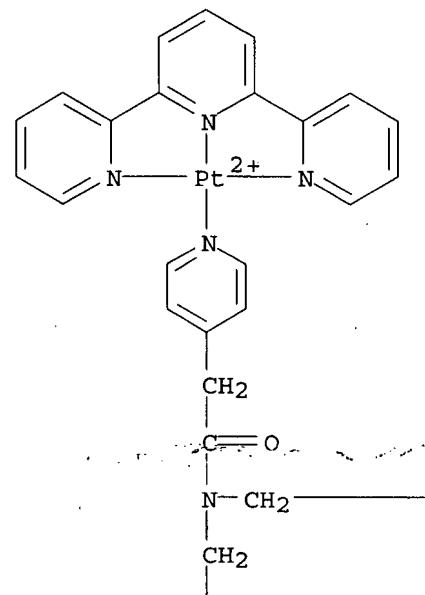
CN Platinum(2+), [N-[2-(benzoylamino)ethyl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycinamide] (2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')-, (SP-4-3)- (9CI) (CA INDEX NAME)



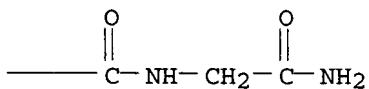
RN 869190-60-3 HCPLUS

CN Platinum(8+), [ $\mu$ 4-[N-[(4-pyridinyl- $\kappa$ N)acetyl]-N-[4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]tetrakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')tetra- (9CI) (CA INDEX NAME)

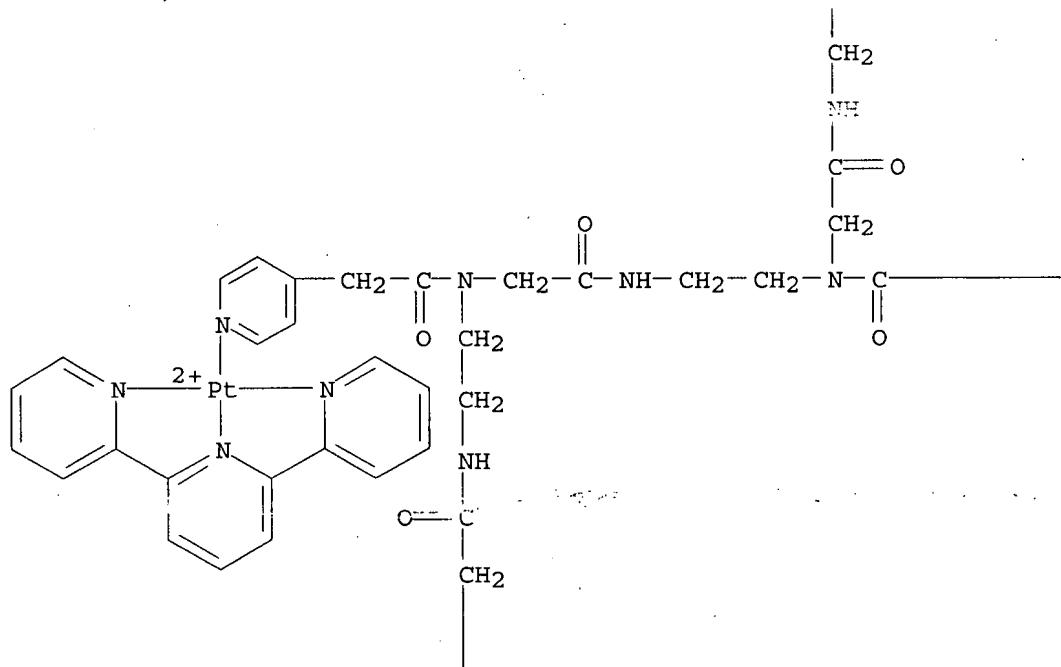
PAGE 1-A



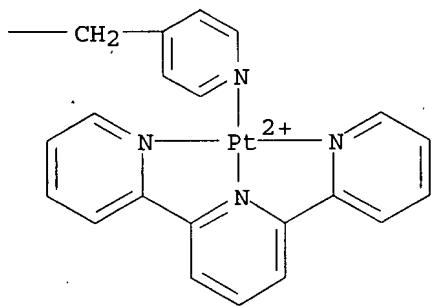
PAGE 1-B



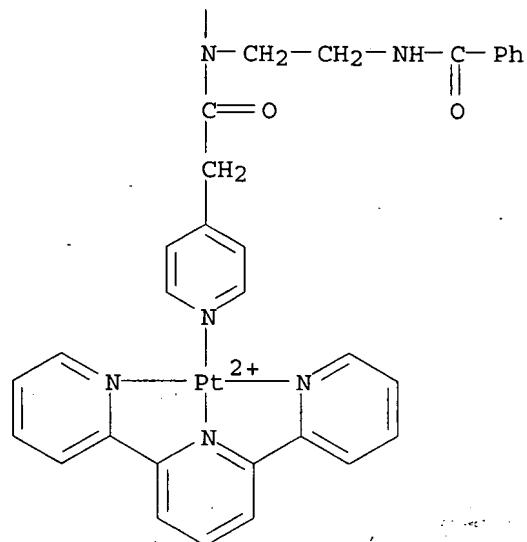
PAGE 2-A



PAGE 2-B



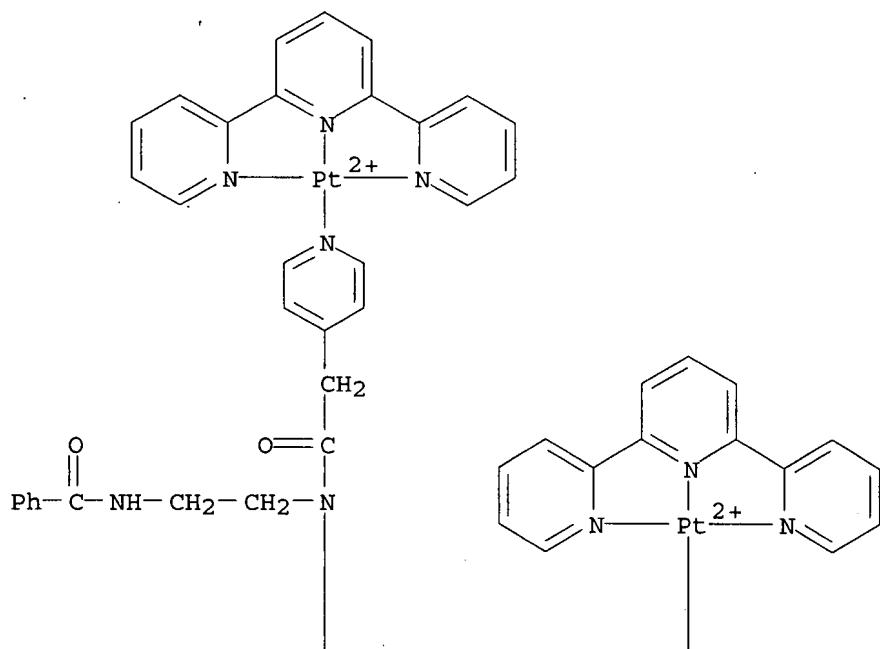
PAGE 3 - A



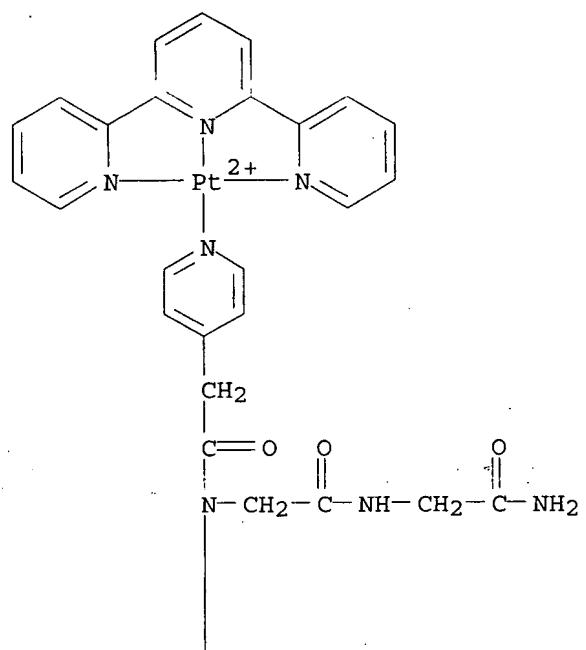
RN 869190-62-5 HCAPLUS

CN Platinum(10+), [ $\mu$ 5-[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaocacos-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycinamide]pentakis(2,2':6',2'''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')pent-(9CI) (CA INDEX NAME)

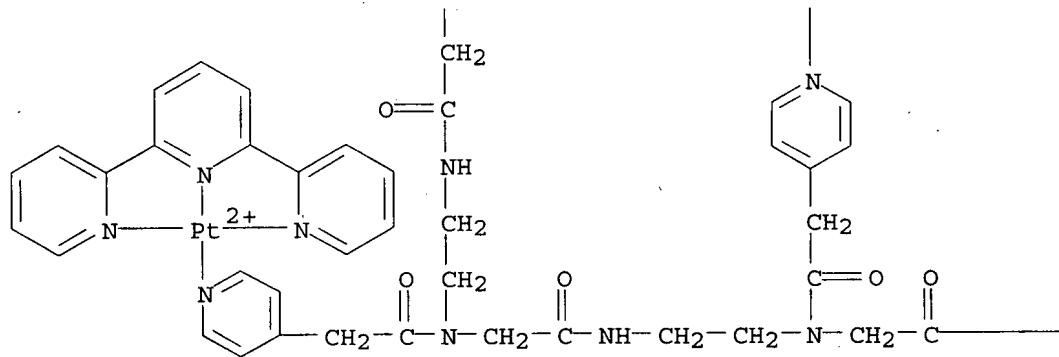
PAGE 1-A



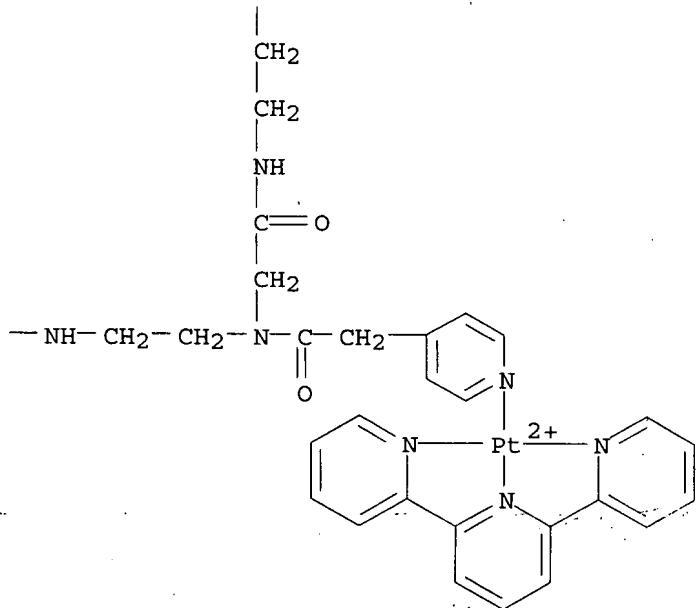
PAGE 1-B



PAGE 2-A



PAGE 2-B

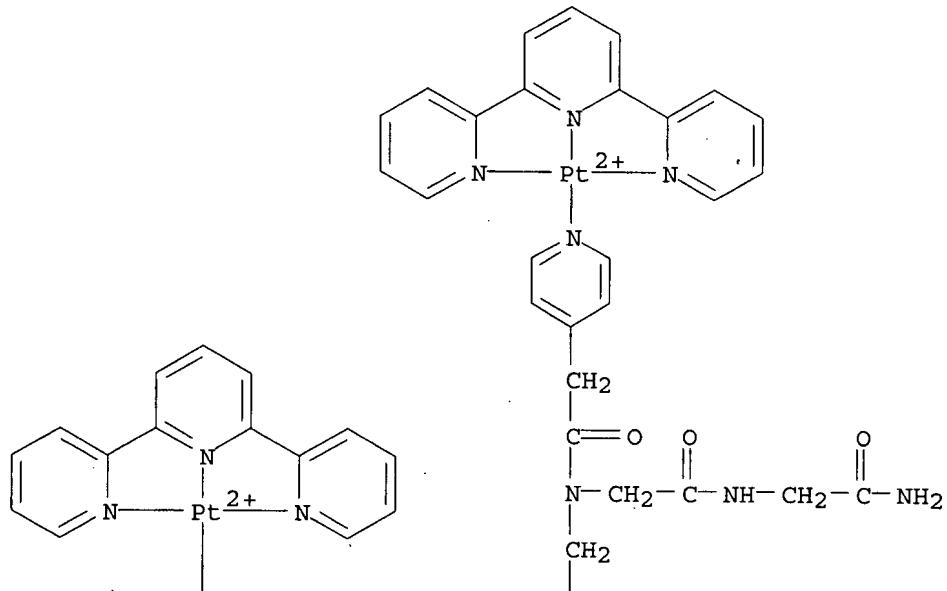


RN 869190-64-7 HCAPLUS

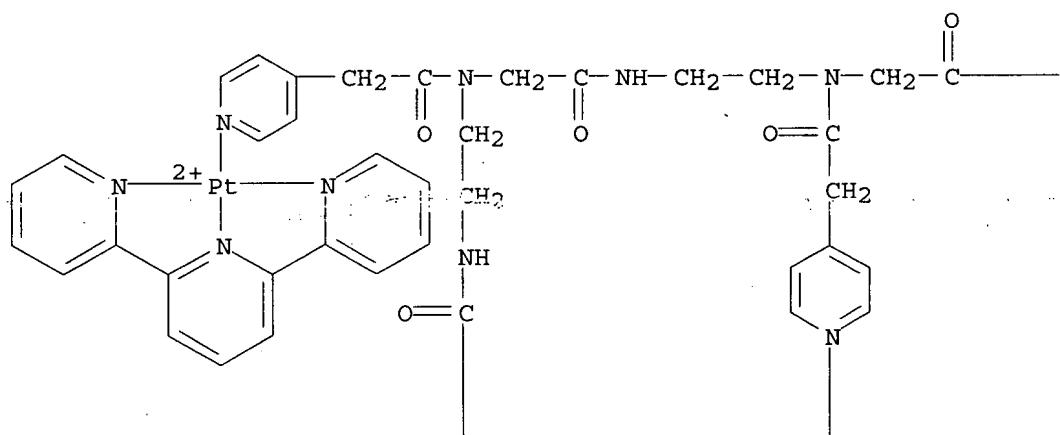
CN Platinum(12+), [ $\mu_6$ -[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycina mide]]hexakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')hexa-

a- (9CI) (CA INDEX NAME)

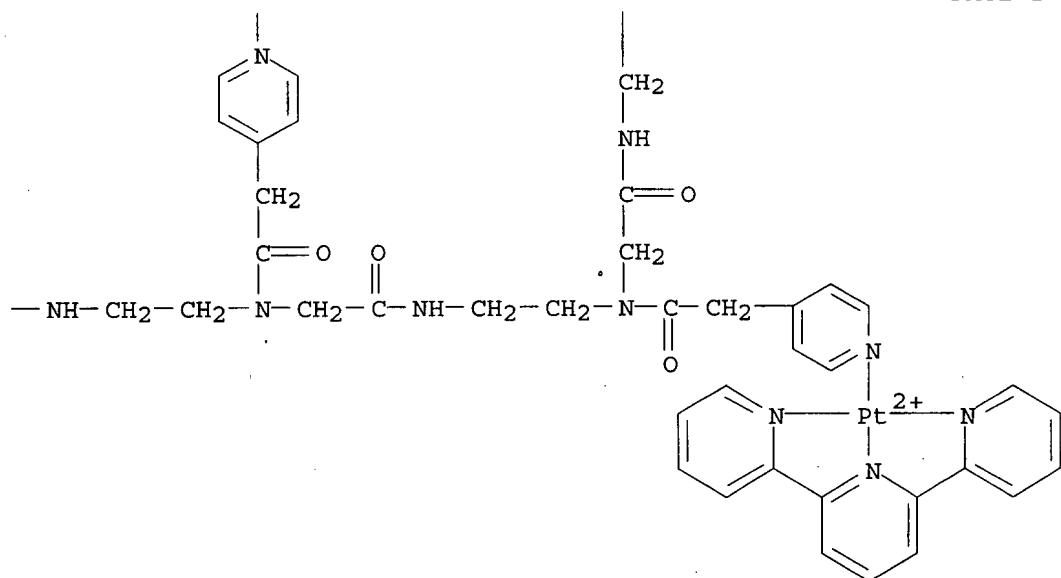
PAGE 1-B



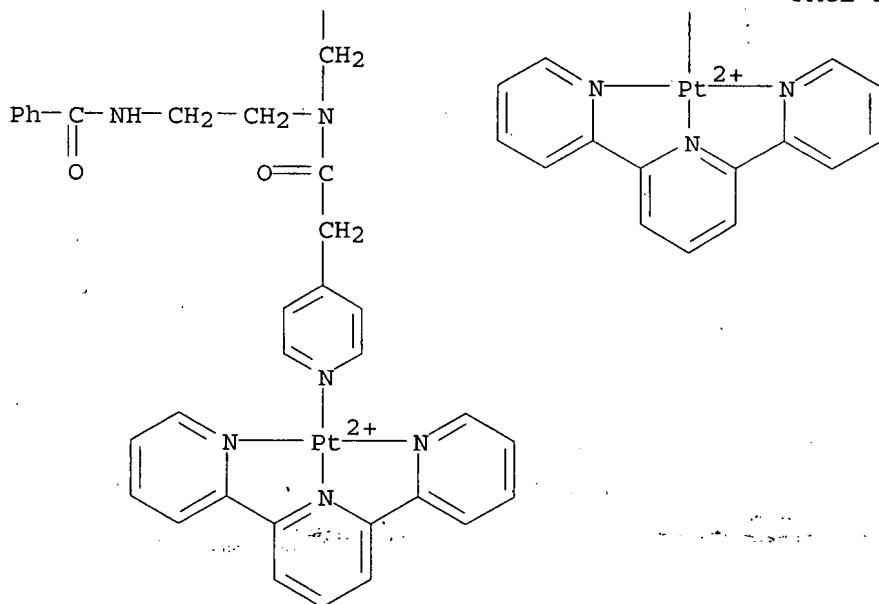
PAGE 2-A



PAGE 2-B



PAGE 3-A



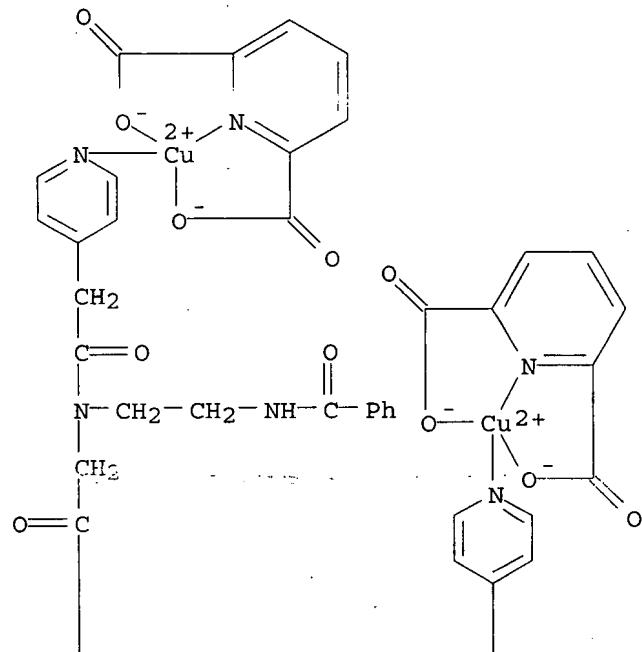
IT 861886-02-4P 861886-04-6P 869190-49-8P  
 869190-50-1P 869190-51-2P 869190-53-4P  
 869190-55-6P 869190-57-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of pyridine-substituted **oligopeptide** scaffolds  
 coordinated with metal(II) chelates)

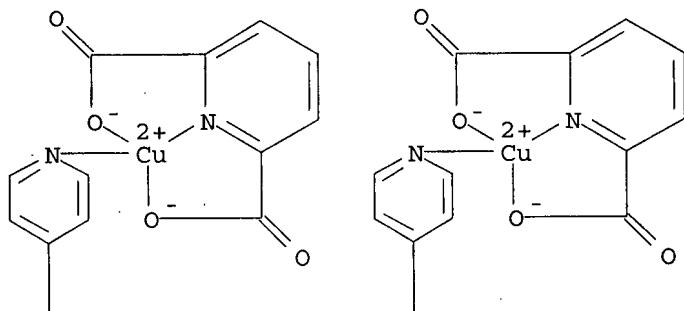
RN 861886-02-4 HCAPLUS

CN Copper, [ $\mu_6$ -[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetracont-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycina mide]]hexakis[2,6-pyridinedicarboxylato(2-)- $\kappa$ N1, $\kappa$ O2, $\kappa$ O6] hexa-, stereoisomer (9CI) (CA INDEX NAME)

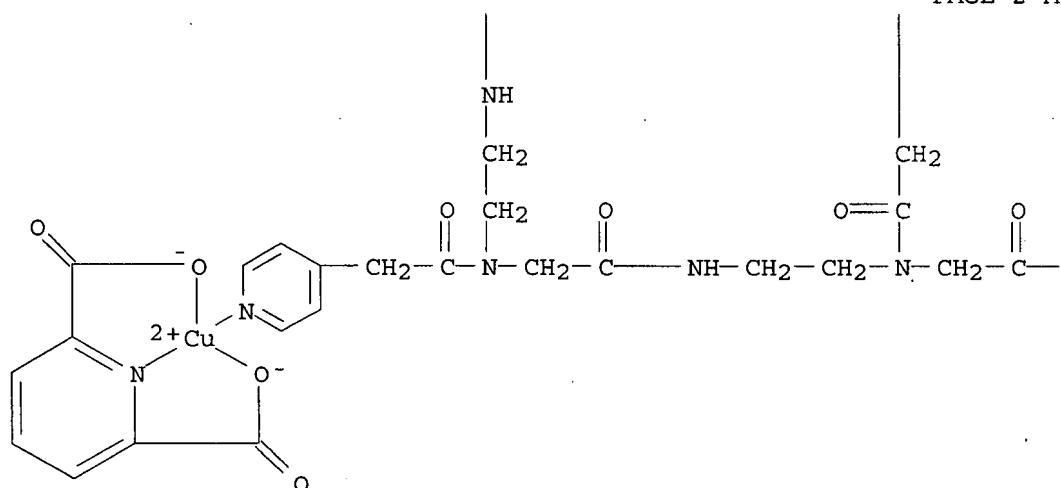
PAGE 1-A



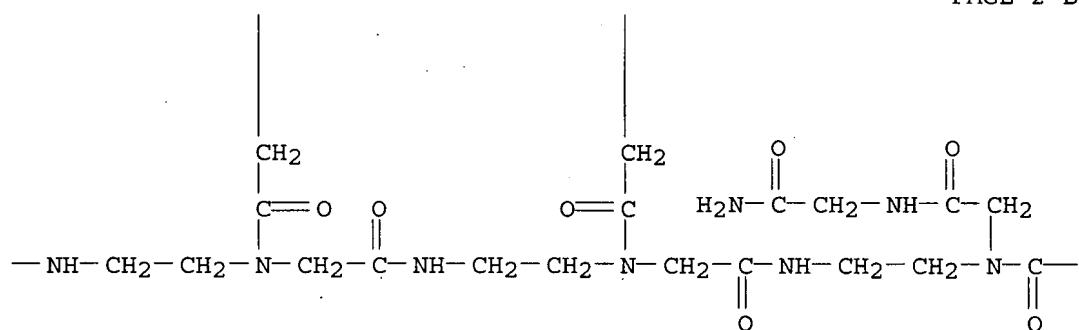
PAGE 1-B



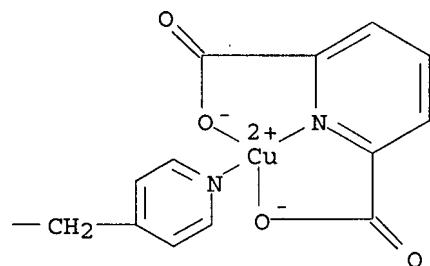
PAGE 2-A



PAGE 2-B



PAGE 2-C



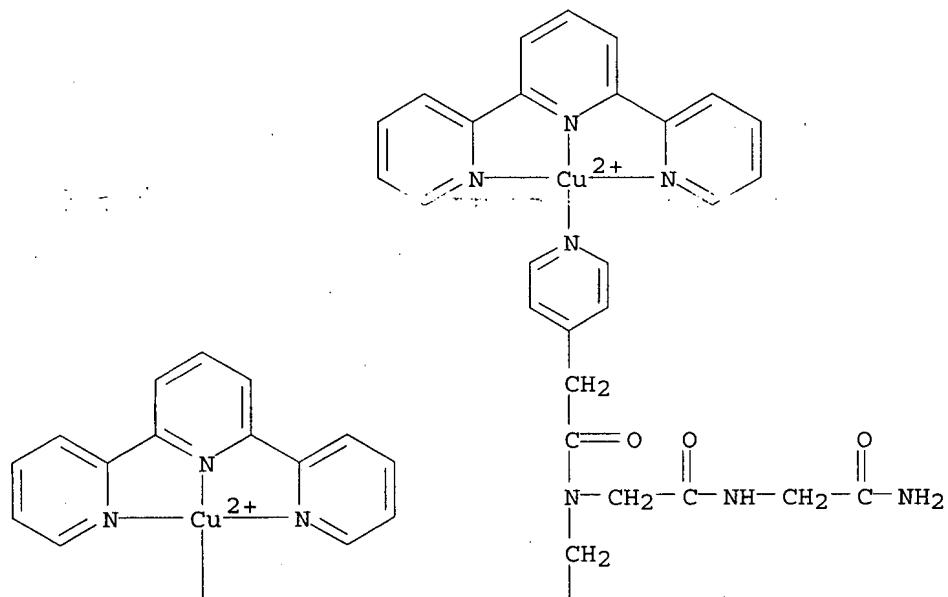
RN 861886-04-6 HCPLUS

CN Copper(12+), [ $\mu$ 6-[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetratriacont-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycina mide]]hexakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')hexa-, stereo-isomer, dodecaperchlorate (9CI) (CA INDEX NAME)

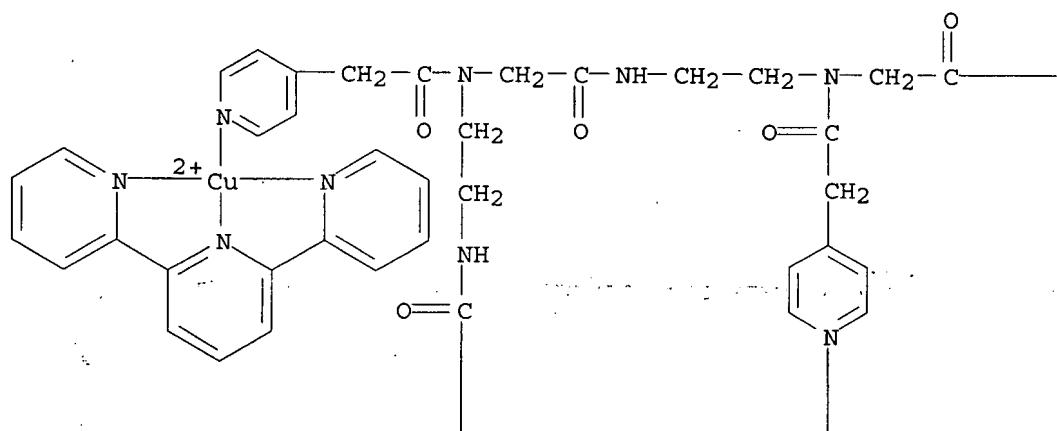
CM 1

CRN 861886-03-5  
CMF C165 H154 Cu6 N38 O14  
CCI CCS

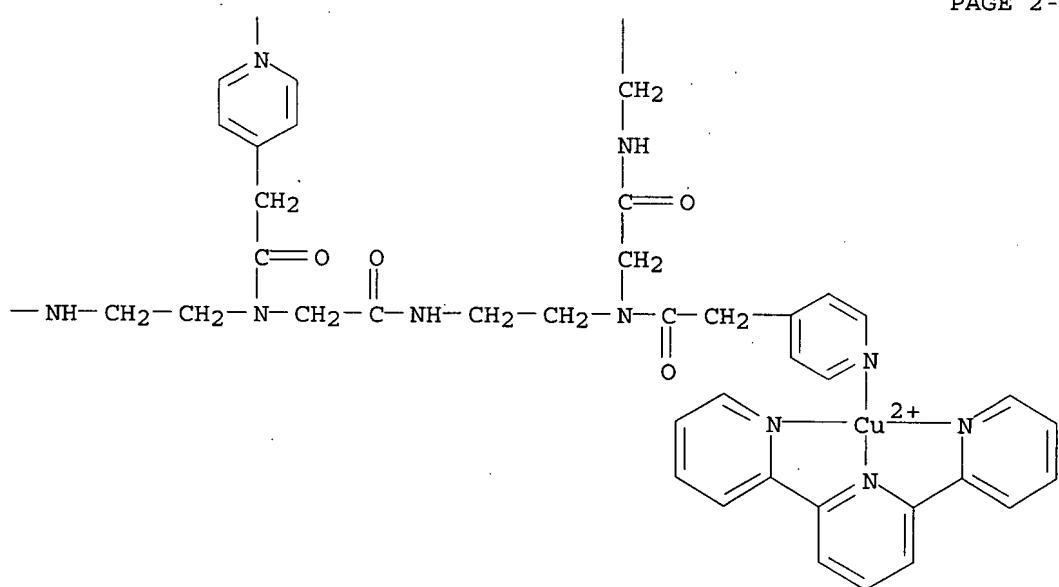
PAGE 1-B



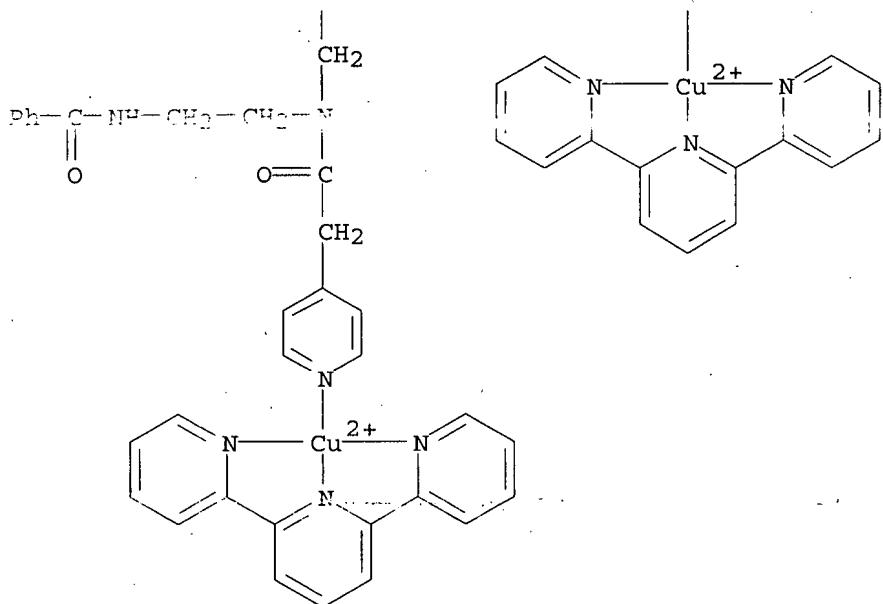
PAGE 2-A



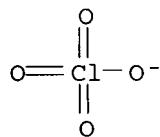
PAGE 2-B



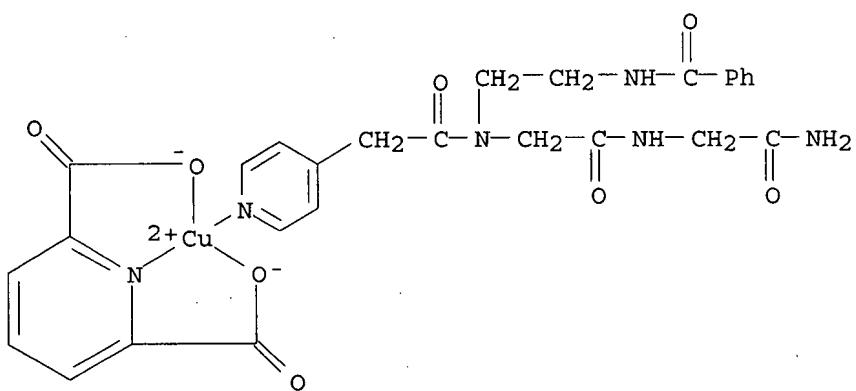
PAGE 3-A



CM 2

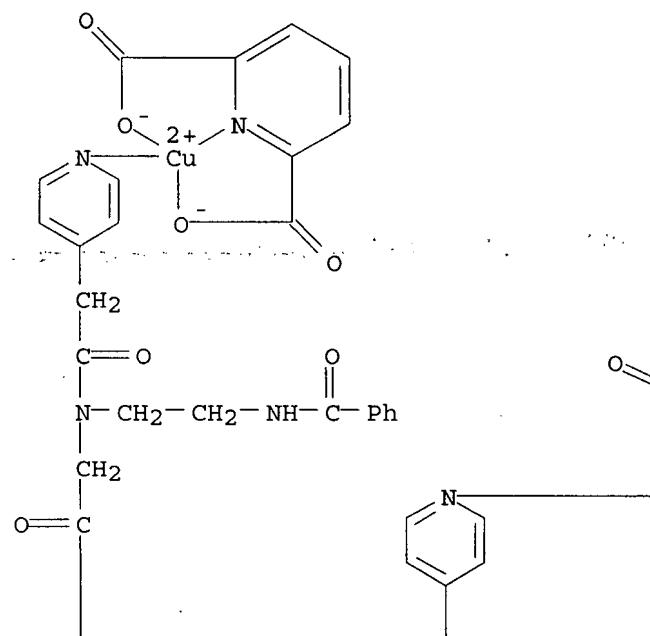
CRN 14797-73-0  
CMF Cl O4

RN 869190-49-8 HCPLUS  
 CN Copper, [N-[2-(benzoylamino)ethyl]-N-[(4-pyridyl-  
 κN)acetyl]glycylglycinamide] [2,6-pyridinedicarboxylato(2-)-  
 κN1,κO2,κO6]-, (SP-4-1)- (9CI) (CA INDEX NAME)

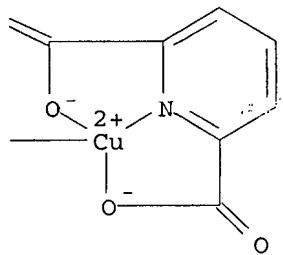


RN 869190-50-1 HCPLUS  
 CN Copper, tetrakis[2,6-pyridinedicarboxylato(2-) -  
 κN1,κO2,κO6] [μ4- [N- [(4-pyridinyl-κN)acetyl]-N-  
 [4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl-κN)acetyl]-  
 3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]tetra-,  
 stereoisomer (9CI) (CA INDEX NAME)

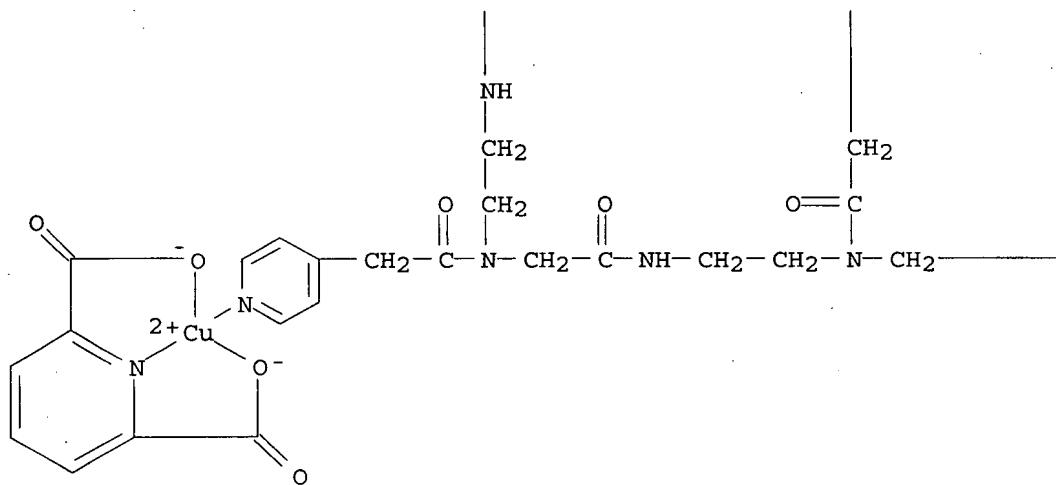
PAGE 1-A



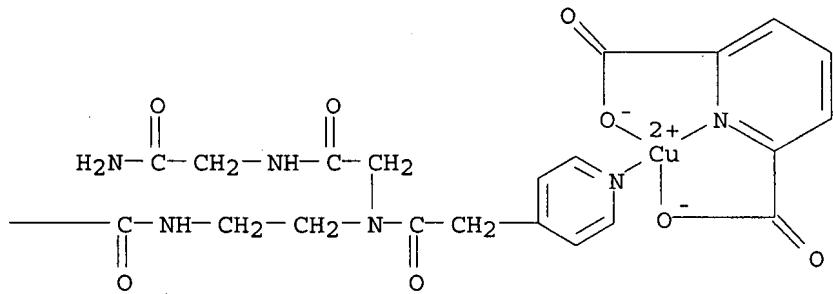
PAGE 1-B



PAGE 2-A



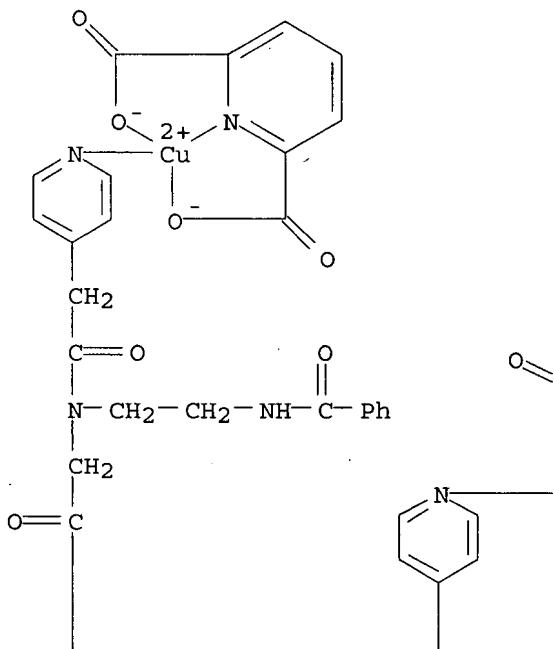
PAGE 2-B



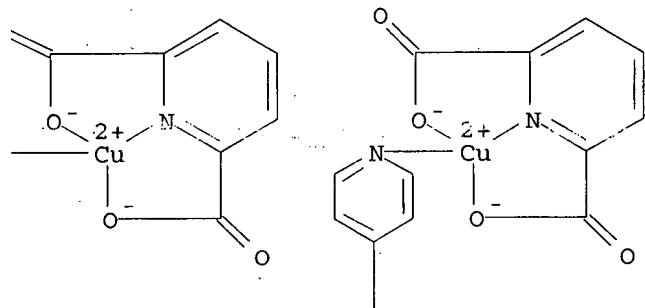
RN 869190-51-2 HCPLUS

CN Copper, [ $\mu$ 5-[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaoctacos-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycinamide]pentakis[2,6-pyridinedicarboxylato(2-)- $\kappa$ N1, $\kappa$ O2, $\kappa$ O6]penta-, stereoisomer (9CI) (CA INDEX NAME)

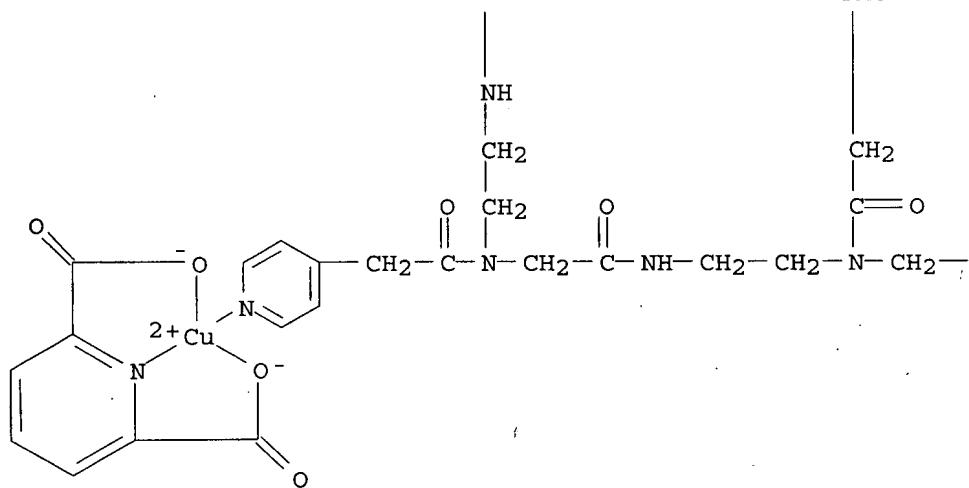
PAGE 1-A



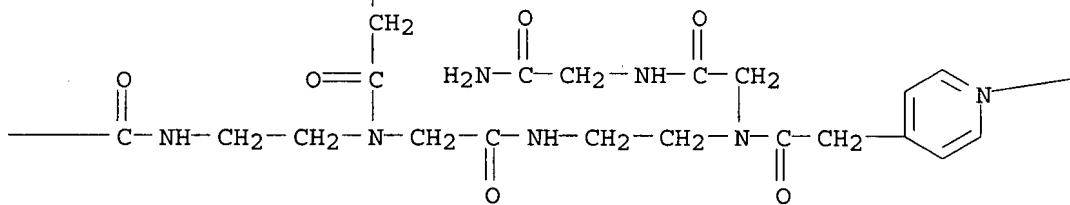
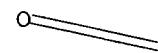
PAGE 1-B



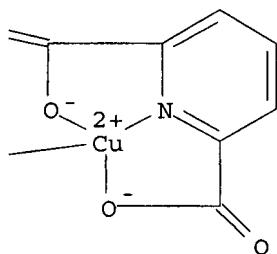
PAGE 2-A



PAGE 2-B



PAGE 2-C



RN 869190-53-4 HCAPLUS

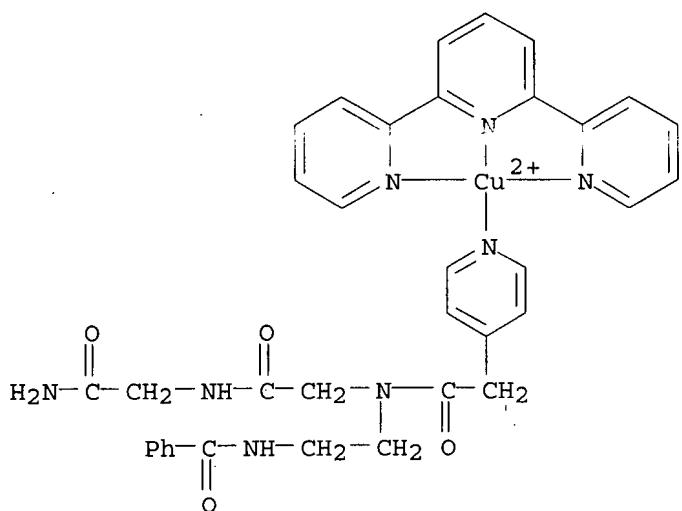
CN Copper (2+), [N- [2- (benzoylamino) ethyl]-N- [(4-pyridinyl-  
 $\kappa N$ ) acetyl]glycylglycinamide] (2,2':6',2''-terpyridine-  
 $\kappa N1,\kappa N1',\kappa N1'')$ -, (SP-4-3)-, diperchlorate (9CI) (CA  
 INDEX NAME)

CM 1

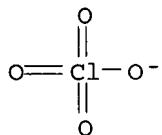
CRN 869190-52-3

CMF C35 H34 Cu N8 O4

CCI CCS



CM 2

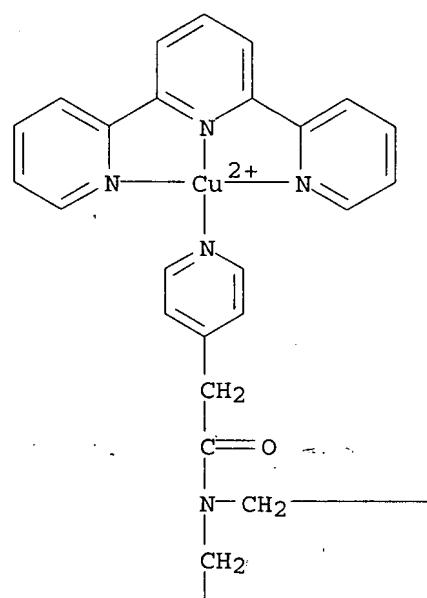
CRN 14797-73-0  
CMF Cl O4

RN 869190-55-6 HCPLUS  
 CN Copper(8+), [ $\mu_4$ -[N-[(4-pyridinyl- $\kappa$ N)acetyl]-N-[4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]]tetrakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')tetra-, stereoisomer, octaperchlorate (9CI) (CA INDEX NAME)

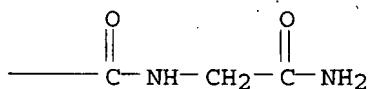
CM 1

CRN 869190-54-5  
CMF C113 H106 Cu4 N26 O10  
CCI CCS

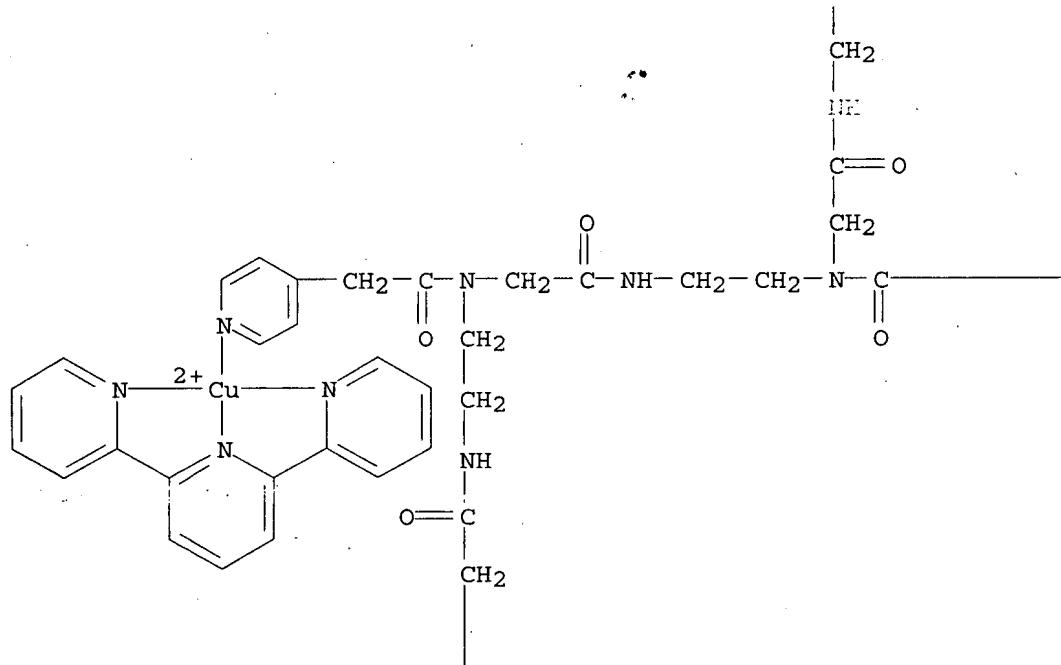
PAGE 1-A



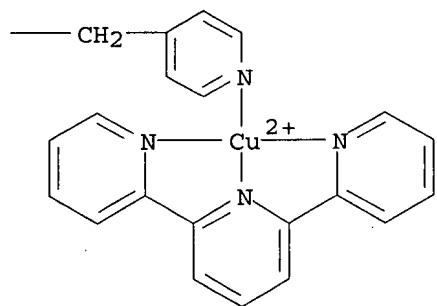
PAGE 1-B



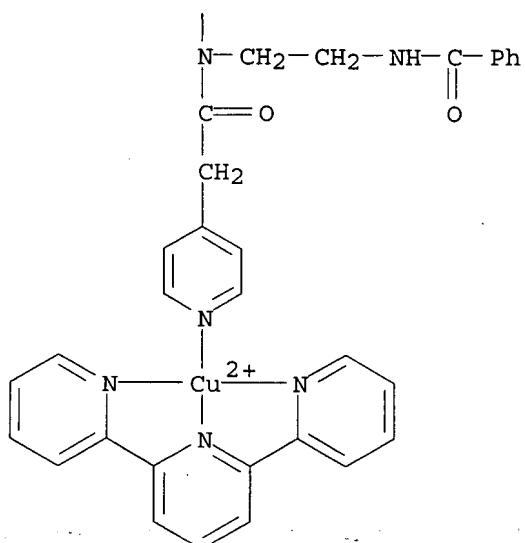
PAGE 2-A



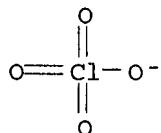
PAGE 2-B



PAGE 3-A



CM 2

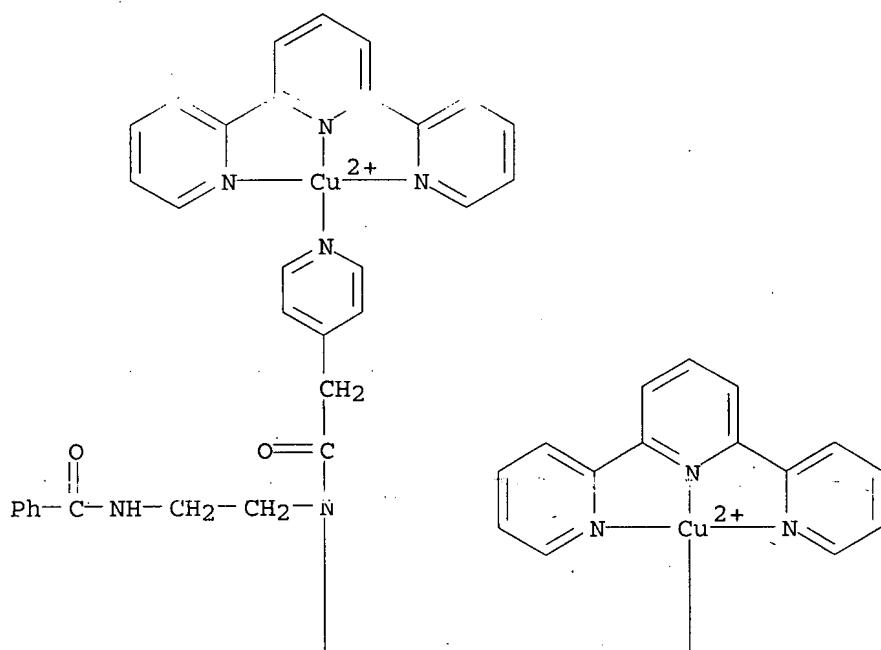
CRN 14797-73-0  
CMF Cl O4

RN 869190-57-8 HCAPLUS  
 CN Copper(10+), [ $\mu_5$ -[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaocacos-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycinamide]]pentakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')penta-, stereoisomer, decaperchlorate (9CI) (CA INDEX NAME)

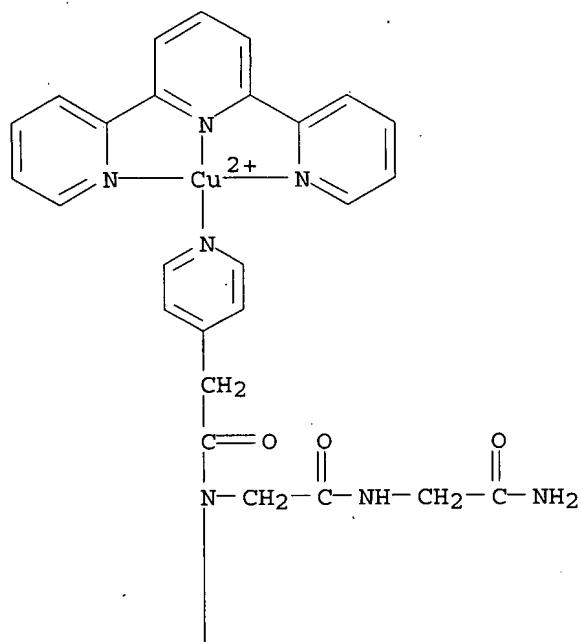
CM 1

CRN 869190-56-7  
CMF C139 H130 Cu5 N32 O12  
CCI CCS

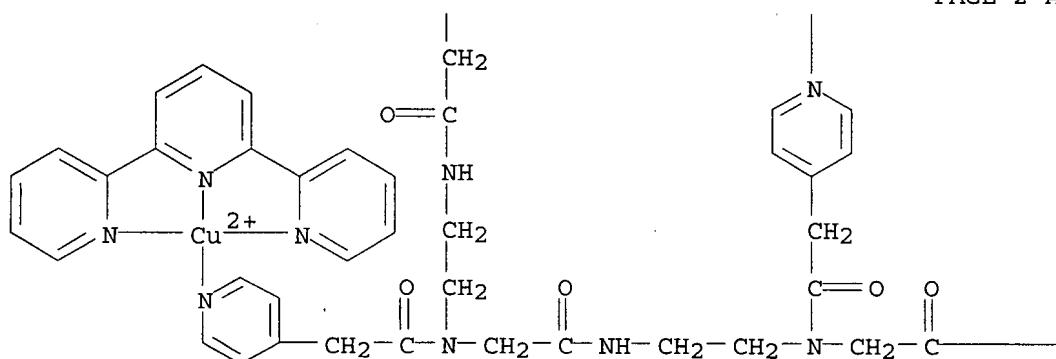
PAGE 1-A



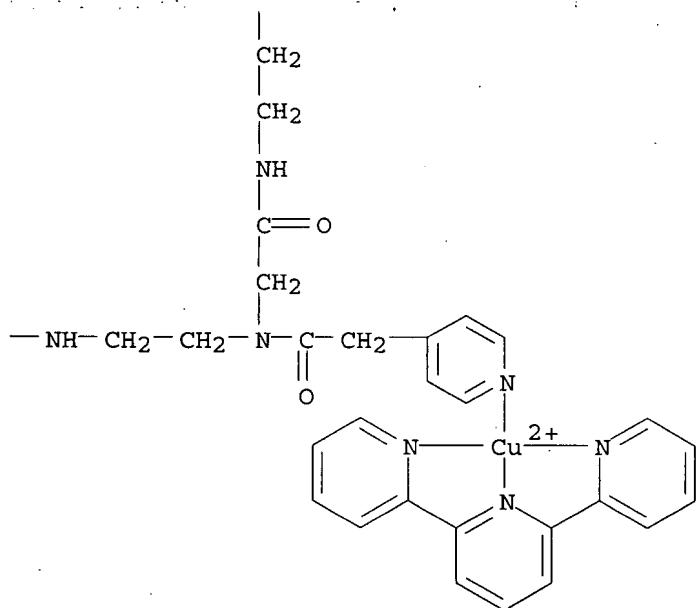
PAGE 1-B



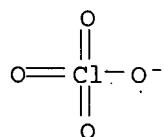
PAGE 2-A



PAGE 2-B



CM 2

CRN 14797-73-0  
CMF Cl O4IT 869190-59-0P 869190-61-4P 869190-63-6P  
869190-65-8P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (preparation, cyclic voltammetry, and diffusion coefficient measured with chronoamperometry)

RN 869190-58-9 INDEX NAME

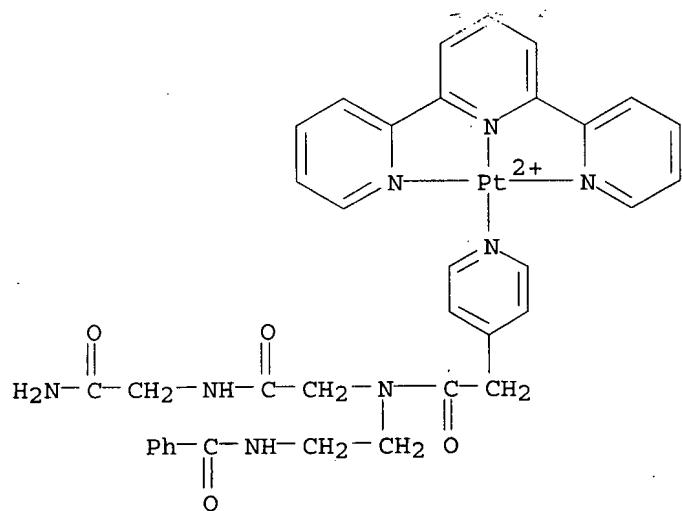
CN Platinum(2+), [N-[2-(benzoylamino)ethyl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycinamide](2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')-, (SP-4-3)-, diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 869190-58-9

CMF C35 H34 N8 O4 Pt

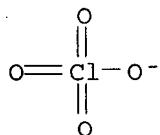
CCI CCS



CM 2

CRN 14797-73-0

CMF Cl O4



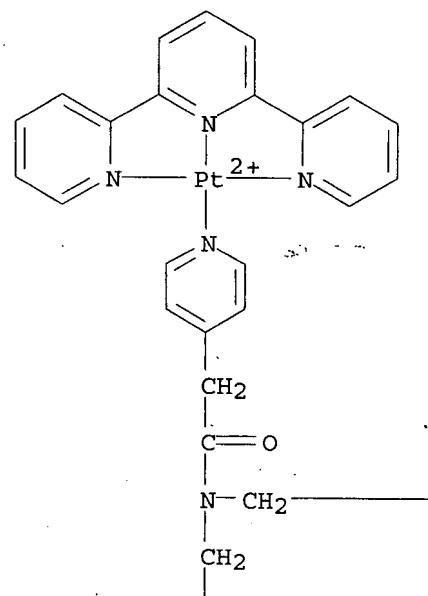
RN 869190-61-4 HCAPLUS

CN Platinum(8+), [ $\mu$ 4-[N-[(4-pyridinyl- $\kappa$ N)acetyl]-N-[4,10,16,22-tetraoxo-22-phenyl-6,12,18-tris[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21-heptaazadocos-1-yl]glycylglycinamide]]tetrakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')tetra-, octaperchlorate (9CI) (CA INDEX NAME)

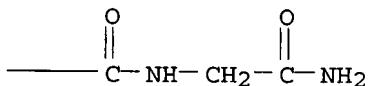
CM 1

CRN 869190-60-3  
CMF C113 H106 N26 O10 Pt4  
CCI CCS

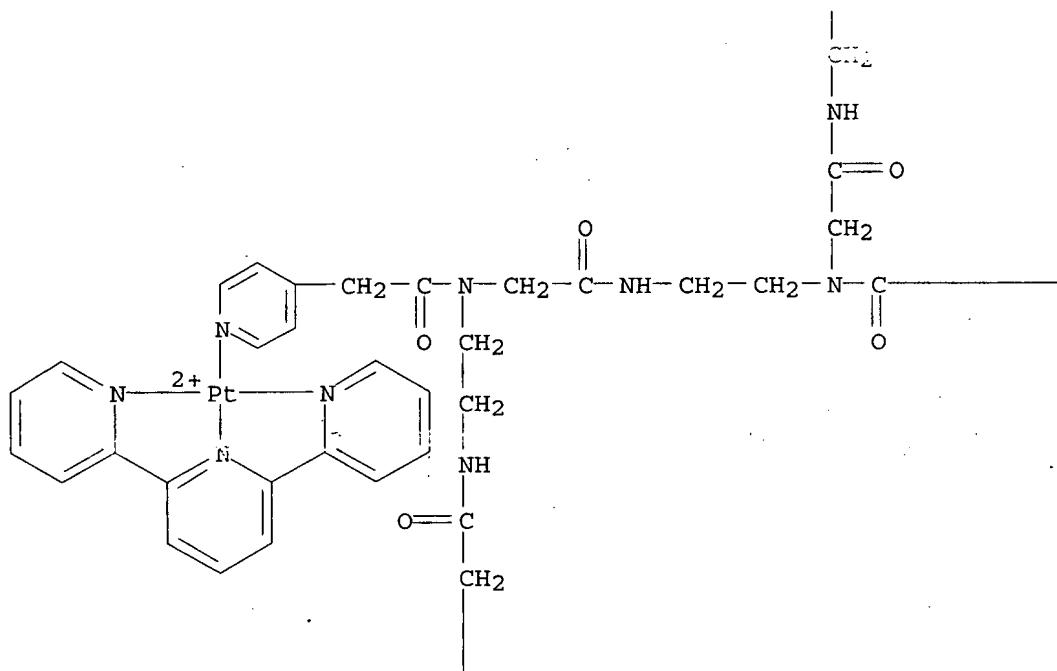
PAGE 1-A



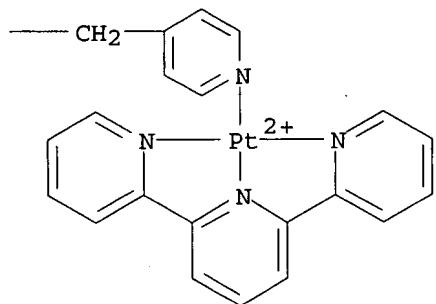
PAGE 1-B



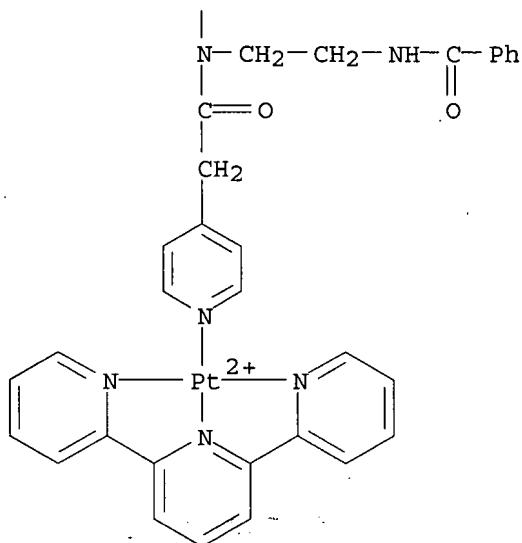
PAGE 2-A



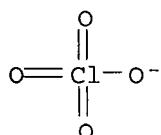
PAGE 2-B



PAGE 3-A



CM 2

CRN 14797-73-0  
CMF Cl O4RN 869190-63-6 HCPLUS  
CN Platinum(10+), [ $\mu_5$ -[N-[4,10,16,22,28-pentaoxo-28-phenyl-6,12,18,24-tetrakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27-nonaazaoctacos-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycinamide]]pentakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')penta-decapерchlorate (9CI) (CA INDEX NAME)

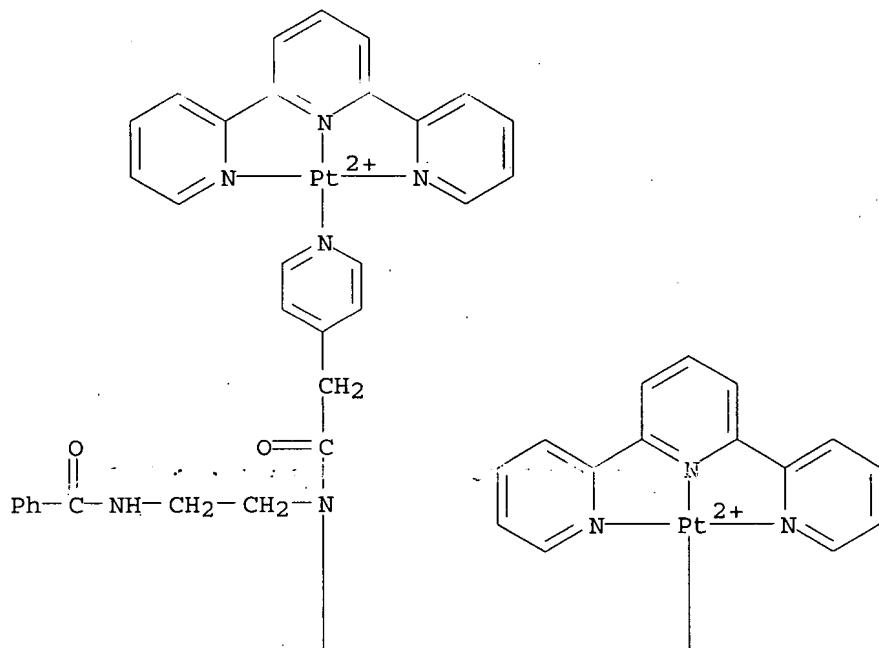
CM 1

CRN 869190-62-5  
CMF C139 H130 N32 O12 Pt5  
CCI CCS

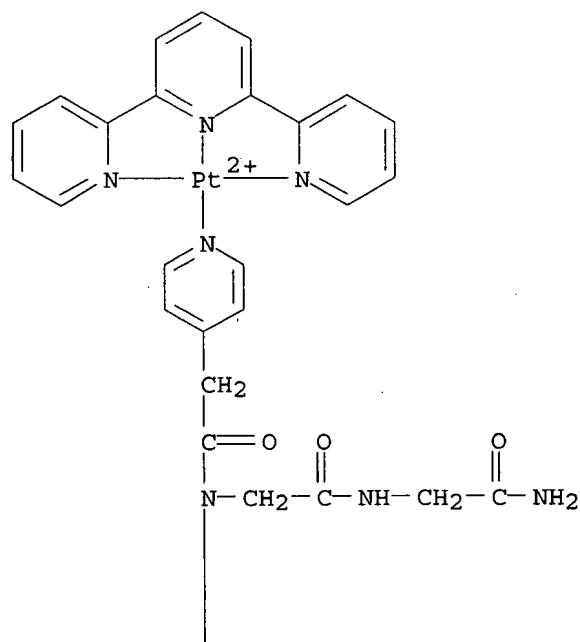
Searched by John DiNatale x2-2557

Page 41

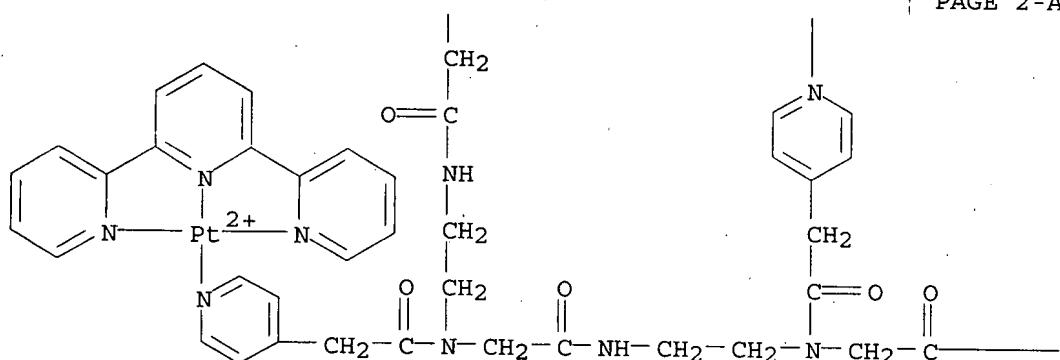
PAGE 1-A



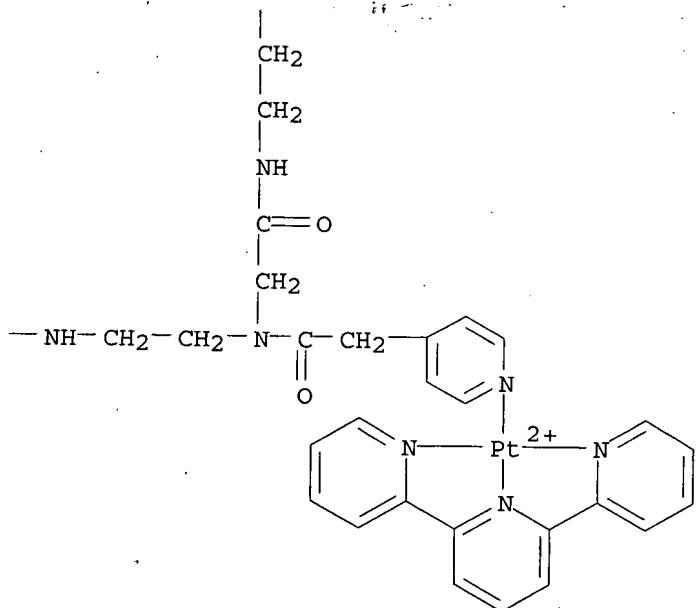
PAGE 1-B



PAGE 2-A

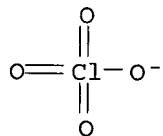


PAGE 2-B



CM 2

CRN 14797-73-0  
CMF Cl O4



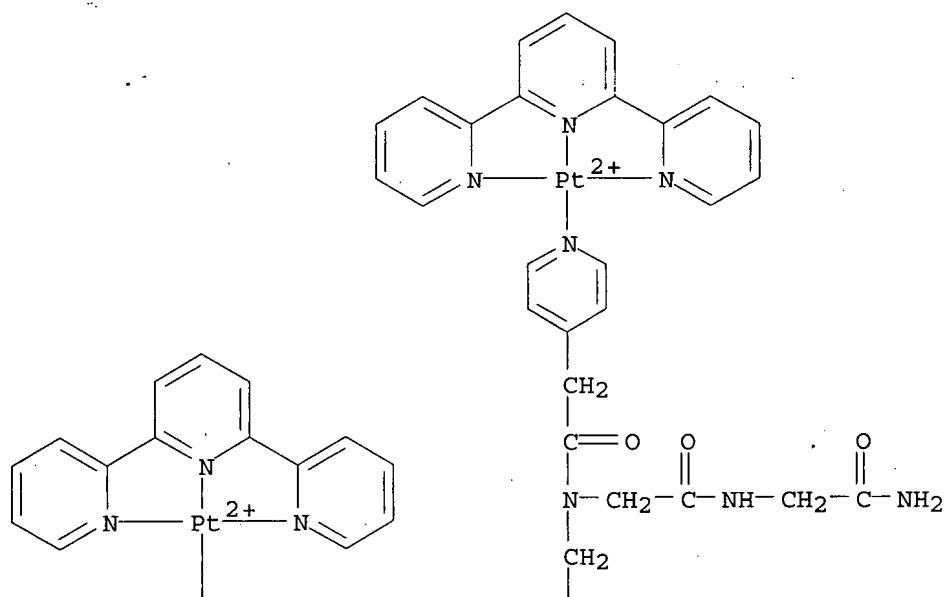
RN 869190-65-8 HCPLUS  
CN Platinum(12+), [μ<sub>6</sub>-[N-[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-

pentakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetracont-1-yl]-N-[{(4-pyridinyl- $\kappa$ N)acetyl]glycylglycine mide}hexakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')hexa-, dodecaperchlorate (9CI) (CA INDEX NAME)

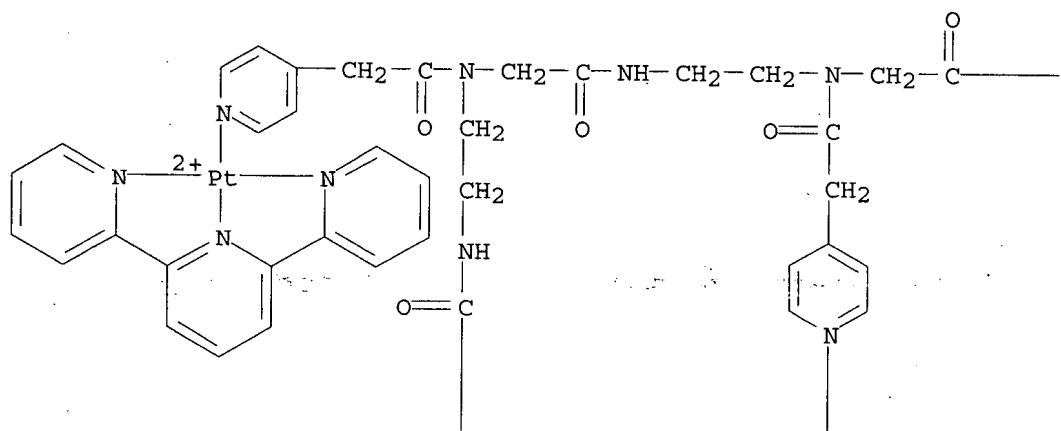
Crn 1

CRN 869190-64-7  
 CMF C165 H154 N38 O14 Pt6  
 CCI CCS

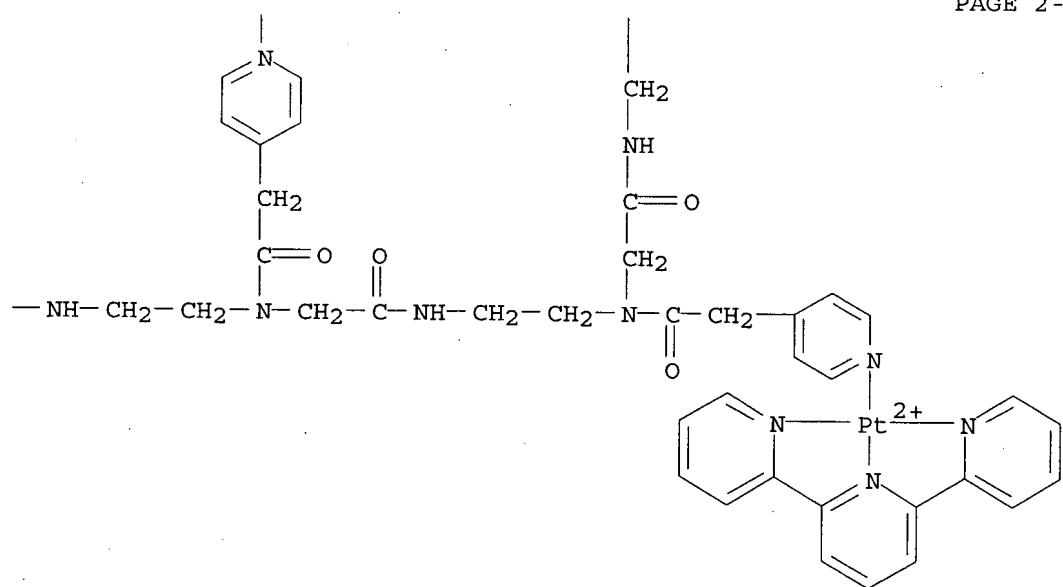
PAGE 1-B



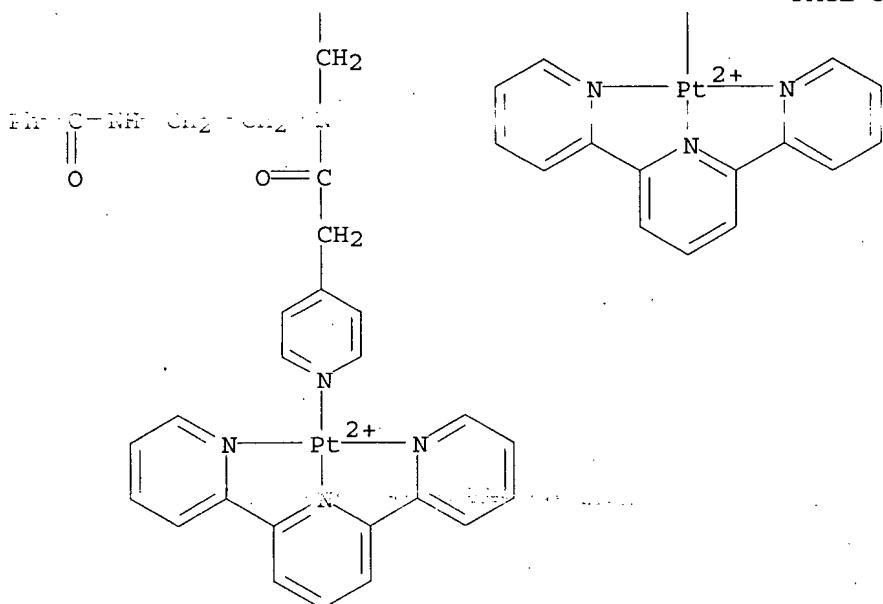
PAGE 2-A



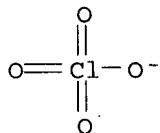
PAGE 2-B



PAGE 3-A



CM 2

CRN 14797-73-0  
CMF Cl O4

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 4 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:508556 HCPLUS  
 DOCUMENT NUMBER: 143:205125  
 TITLE: Artificial Oligopeptide Scaffolds for Stoichiometric Metal Binding  
 AUTHOR(S): Gilmartin, Brian P.; Ohr, Kristi; McLaughlin, Rebekah L.; Koerner, Richard; Williams, Mary Elizabeth  
 CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA  
 SOURCE: Journal of the American Chemical Society (2005), 127(26), 9546-9555  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 143:205125  
 AB Two artificial peptides with pendant pyridine or bipyridine ligands were synthesized and incorporated into oligomeric strands that are

analogous to **peptide** nucleic acid. Spectrophotometric titrns. with Cu<sup>2+</sup> and Fe<sup>2+</sup> show that the oligomers bind stoichiometric quantities of **transition metals** based on the number of pendant ligands. The identities of the titration products are confirmed by high resolution **mass spectrometry**. In the case of the bipyridine **tripeptides**, the titration stoichiometry and mass spectra indicate that the metal ions form interstrand cross-links between two **oligopeptides**, creating duplex structures linked exclusively by metal ions. Calculated mol. structures of the metalated **oligopeptides** and duplexes indicate that the **peptide** backbone acts as a scaffold for the directed assembly of metal ions. ESR spectroscopy of the Cu-containing mols. have varying degrees of electronic interaction based on their charge and supramol. structure. Cyclic voltammetry of the Fe<sup>2+</sup>- and Cu<sup>2+</sup>-linked bpy **oligopeptide** duplexes shows that they possess unique electrochem. signatures based on the redox reactivity of the metal complex.

CC 78-7 (Inorganic Chemicals and Reactions)  
 ST Section cross-reference(s): 34, 72, 77  
 oligopeptide scaffold prepn stoichiometric complexation transition metal; copper artificial **oligopeptide**  
 scaffold prepn EPR cyclic voltammetry; iron artificial **oligopeptide** scaffold prepn cyclic voltammetry; mol structure calcn copper **oligopeptide** scaffold complex  
 IT Redox reaction  
 (electrochem.; of copper(II) and iron(II) complexes of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands)  
 IT Molecular structure  
 (energy-minimized; of hexanuclear copper(II) pyridinedicarboxylate **hexapeptide** complex and bipyridine **tripeptide** duplex from mol. modeling)  
 IT ESR (electron spin resonance)  
 (of copper(II) complexes of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands)  
 IT Molecular modeling  
 (of hexanuclear copper(II) pyridinedicarboxylate **hexapeptide** complex and bipyridine **tripeptide** duplex)  
 IT Transition metal complexes  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (peptide; preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))  
 IT Oligopeptides  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))  
 IT Oligopeptides  
 Peptides, preparation  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (transition metal complexes; preparation of artificial **oligopeptide** scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))  
 IT 6622-91-9, 4-Pyridylacetic acid hydrochloride  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of **hexapeptide** bearing pyridines)  
 IT 861885-96-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)  
 (for preparation of hexapeptide bearing pyridines and subsequent binding to transition metal ions)

IT 169396-88-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of oligopeptides bearing pyridines or bipyridines and subsequent binding to transition metal ions)

IT 118724-25-7, 4'-Methyl-2,2'-bipyridine-4-acetic acid  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (for preparation of tripeptide bearing bipyridines and subsequent binding to transition metal ions)

IT 861885-97-4P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (for preparation of tripeptide bearing bipyridines and subsequent binding to transition metal ions)

IT 861886-05-7P 861886-06-8P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (preparation of artificial oligopeptide scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

IT 861886-02-4P 861886-04-6P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of artificial oligopeptide scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

IT 93-97-0, Benzoic anhydride 29022-11-5, Fmoc-Gly-OH 105047-45-8  
 160400-58-8 861886-00-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of artificial oligopeptide scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

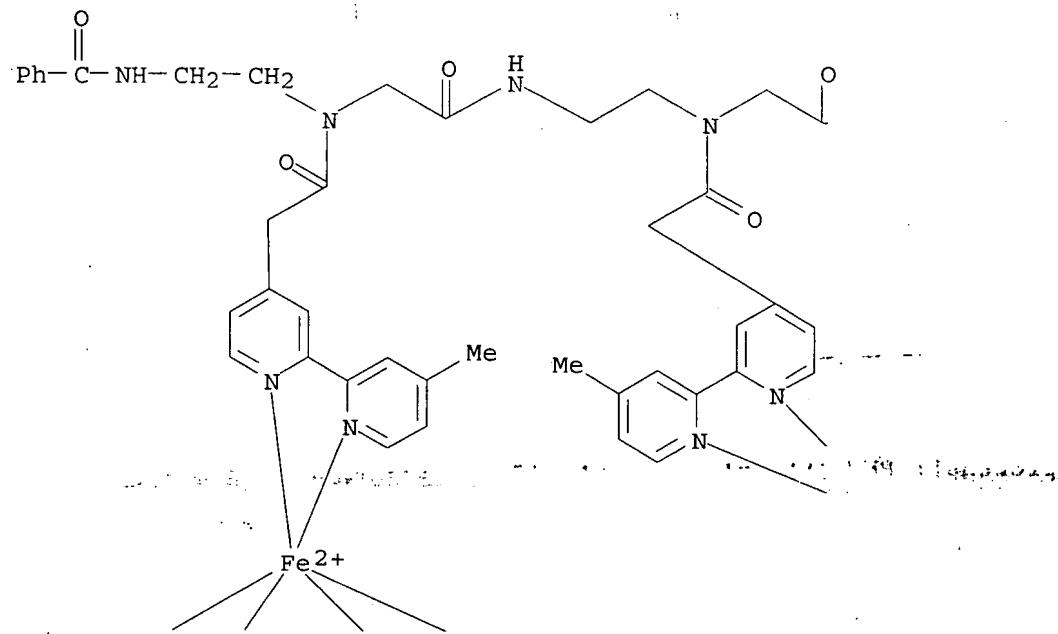
IT 7439-89-6DP, Iron, dinuclear duplex complex of tripeptide with pendant bipyridines 7440-50-8DP, Copper, trinuclear duplex complex of tripeptide with pendant bipyridines 861885-98-5P  
 861885-99-6DP, copper(II) and iron(II) duplex complexes 861885-99-6P  
 861886-01-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of artificial oligopeptide scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

IT 861886-05-7P 861886-06-8P  
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
 (preparation of artificial oligopeptide scaffolds with pendant pyridine or bipyridine ligands for stoichiometric metal binding with copper(II) and iron(II))

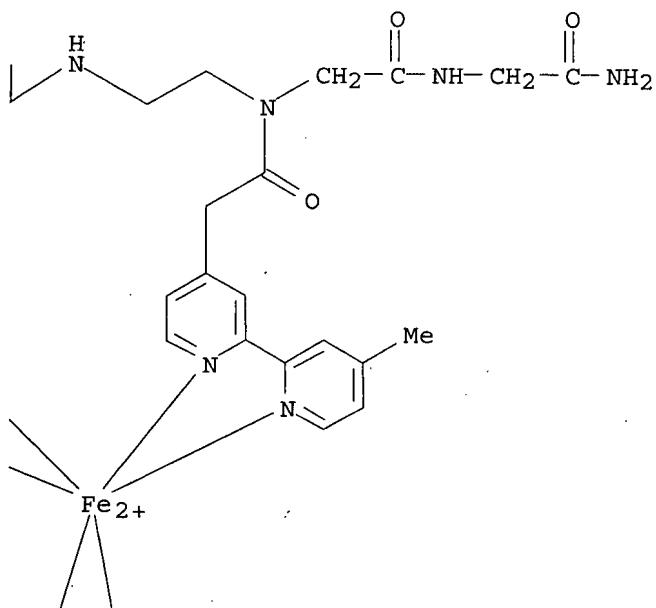
RN 861886-05-7 HCPLUS

CN Iron(4+), bis[ $\mu$ -[N-[6,12-bis[(4'-methyl[2,2'-bipyridin]-4-yl- $\kappa$ N1, $\kappa$ N1')acetyl]-4,10,16-trioxo-16-phenyl-3,6,9,12,15-pentaazahexadec-1-yl]-N-[(4'-methyl[2,2'-bipyridin]-4-yl- $\kappa$ N1, $\kappa$ N1')acetyl]glycylglycinamide]di- (9CI) (CA INDEX NAME)

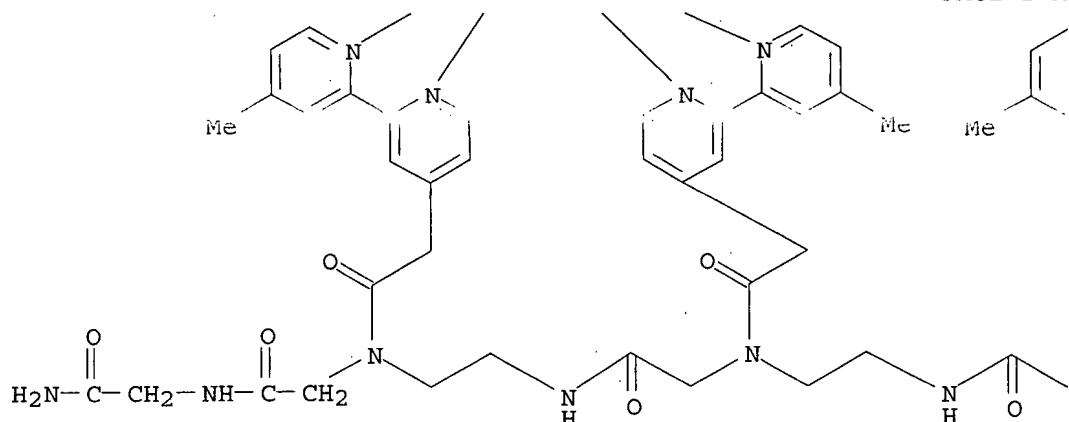
PAGE 1-A



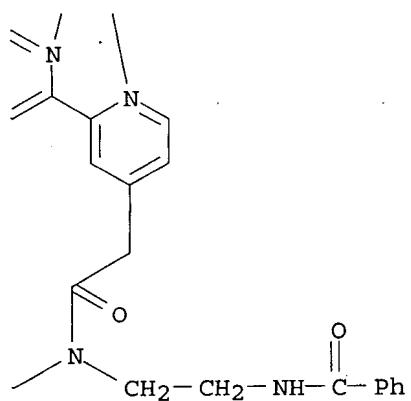
PAGE 1-B



PAGE 2-A

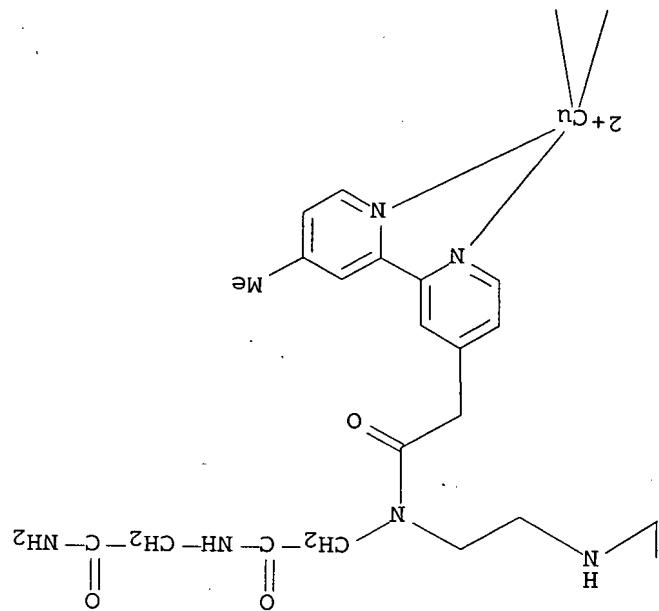


PAGE 2-B

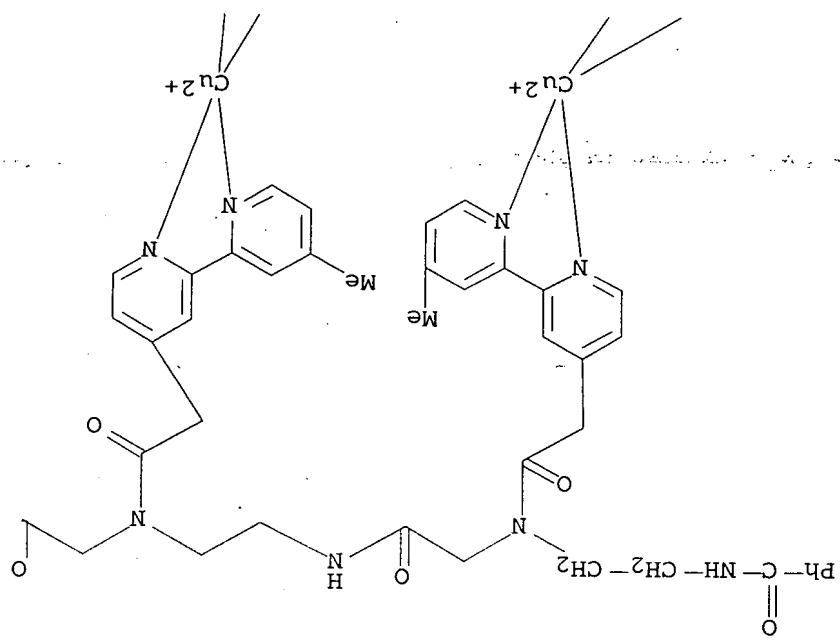


RN 861886-06-8 HCPLUS

CN Copper(6+), bis[μ<sub>3</sub>-[N-[6,12-bis[(4'-methyl[2,2'-bipyridin]-4-yl-κN<sub>1</sub>,κN<sub>1</sub>')acetyl]-4,10,16-trioxo-16-phenyl-3,6,9,12,15-pentaazahexadec-1-yl]-N-[(4'-methyl[2,2'-bipyridin]-4-yl-κN<sub>1</sub>,κN<sub>1</sub>')acetyl]glycylglycinamide]tri-, stereoisomer (9CI)  
(CA INDEX NAME)

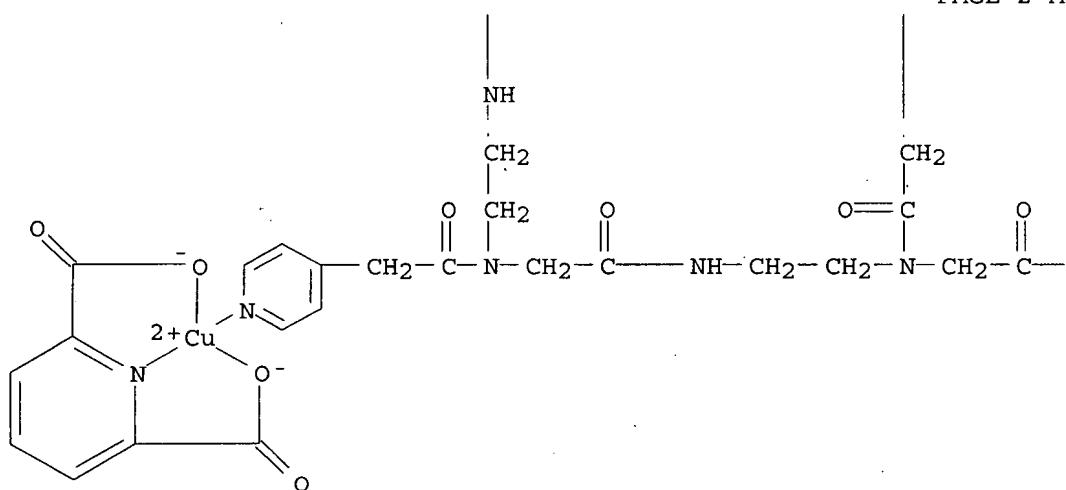


PAGE 1-B

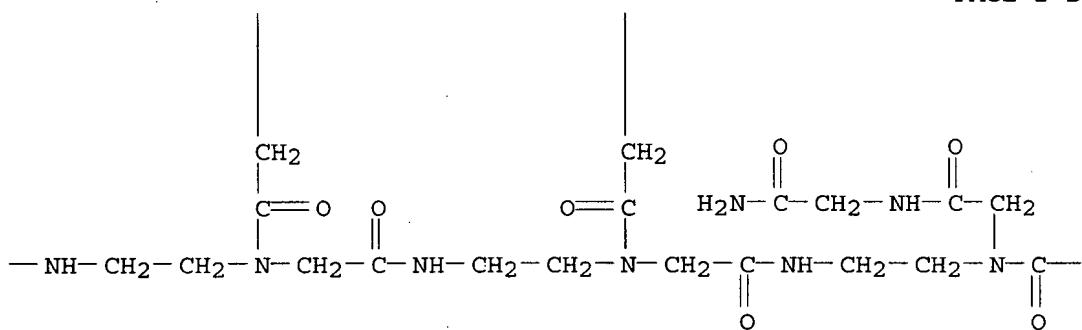


PAGE 1-A

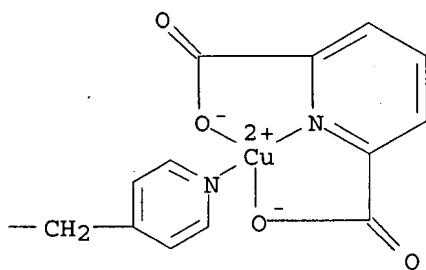
PAGE 2-A



PAGE 2-B

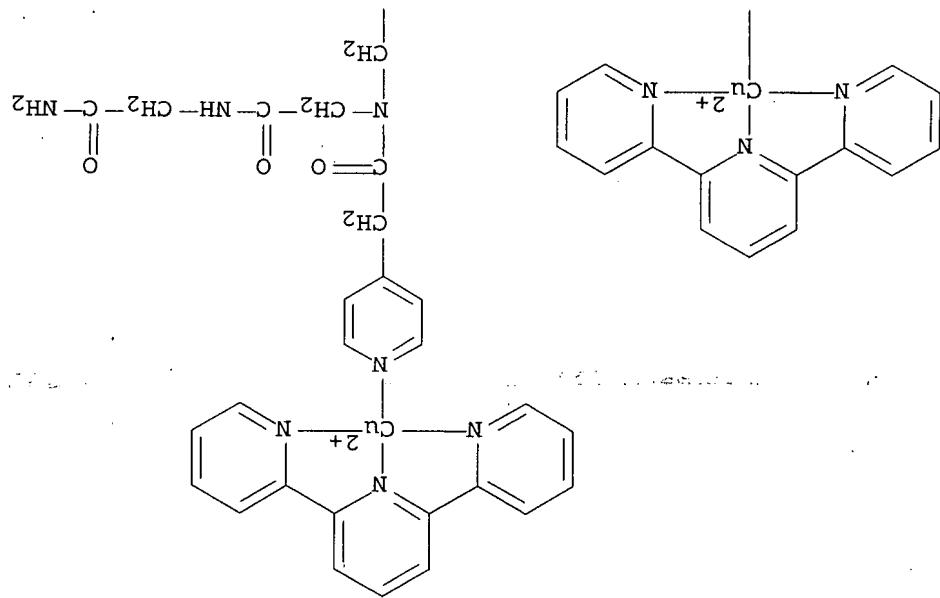


PAGE 2-C



RN 861886-04-6 HCAPLUS

CN Copper(12+), [ $\mu_6$ -[4,10,16,22,28,34-hexaoxo-34-phenyl-6,12,18,24,30-pentakis[(4-pyridinyl- $\kappa$ N)acetyl]-3,6,9,12,15,18,21,24,27,30,33-undecaazatetracont-1-yl]-N-[(4-pyridinyl- $\kappa$ N)acetyl]glycylglycine mide]]hexakis(2,2':6',2''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')hexa-, stereoisomer, dodecaperchlorate (9CI) (CA INDEX NAME)



PAGE 1-B

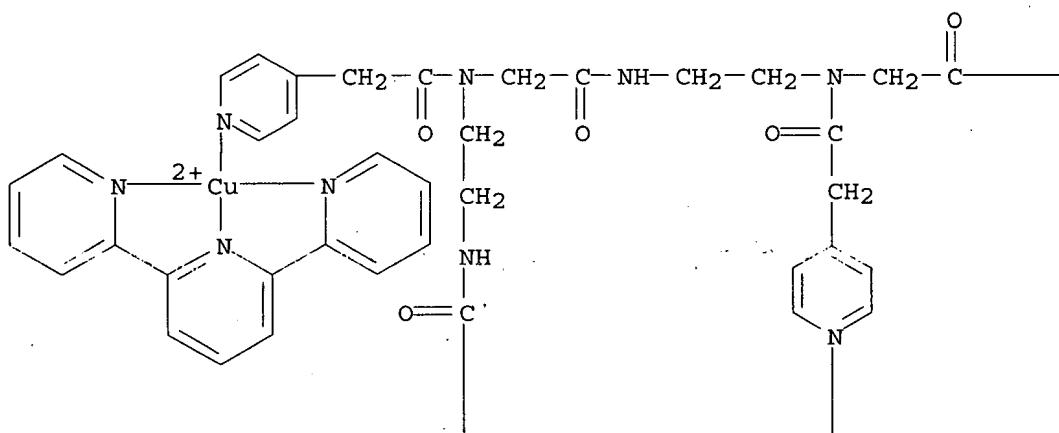
|     |  |  |  |
|-----|--|--|--|
| CRN | 861886-03-5                                    | CCl  | CCl  |
| CMF | C <sub>16</sub> H <sub>15</sub> N <sub>3</sub> | Cu <sub>6</sub> N <sub>3</sub> S <sub>0.14</sub> | Cu <sub>6</sub> N <sub>3</sub> S <sub>0.14</sub> |

CM 1

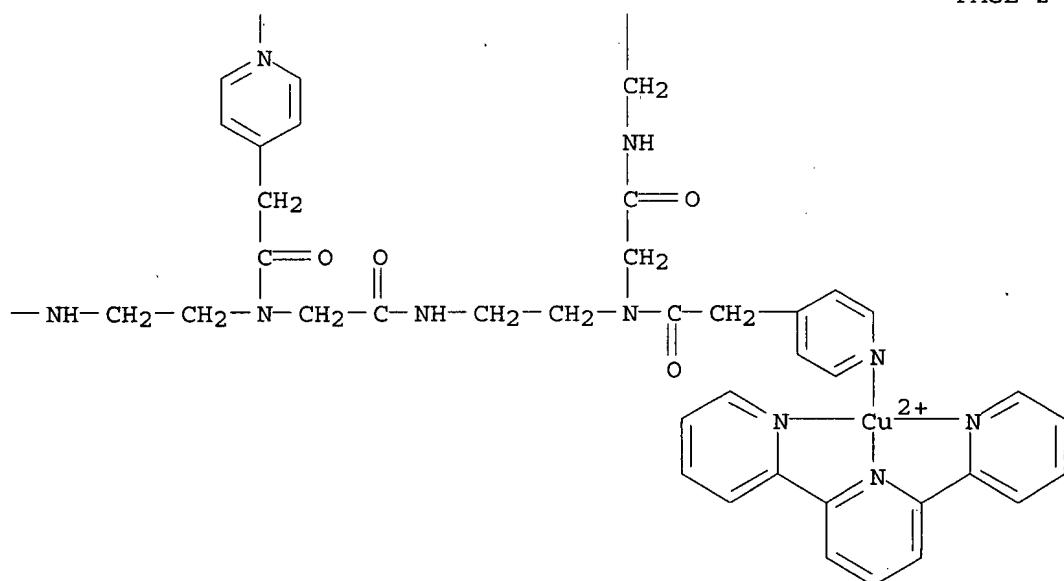
07/20/2006

SRIVASTAVA 10/614324

PAGE 2-A



PAGE 2-B



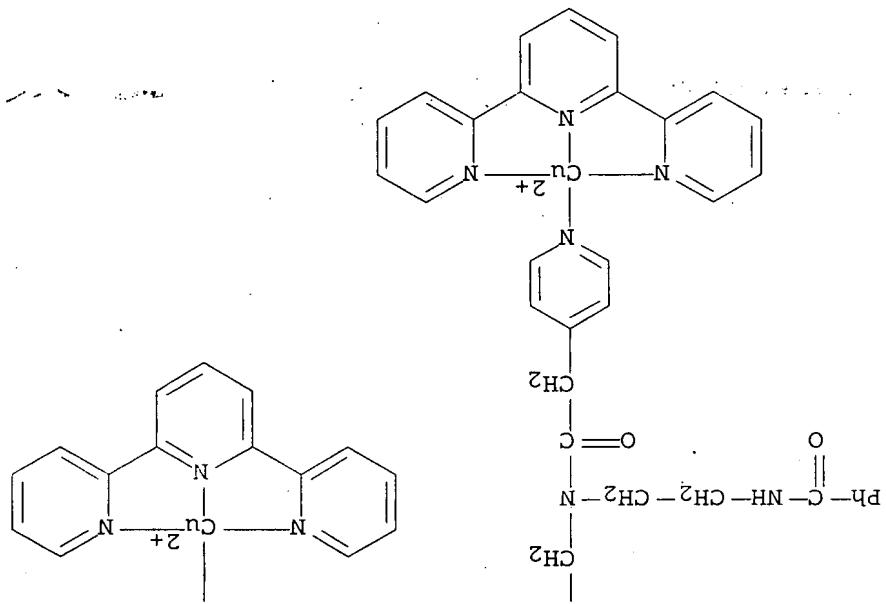
L74 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:438295 HCAPLUS  
 DOCUMENT NUMBER: 143:358931  
 TITLE: Probing the stability and structure of metalloporphyrin complexes with basic peptides  
 AUTHOR(S): Jelleen, Emily E.; Ryzchov, Victor  
 CORPORATE SOURCE: Department of Chemistry and Biochemistry, Northern Illinois University, Dekalb, IL 60115, USA  
 SOURCE: European Journal of Mass Spectrometry (2005), 11(1), 65-72  
 CODEN: EJMSCL ISSN: 1469-0667  
 PUBLISHER: IM Publications  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ABSTRACT: The stability and structure of noncovalent complexes of various  
 peptides containing basic amino acid residues (Arg, Lys) with  
 metalloporphyrins were studied in a quadrupole ion trap mass  
 spectrometer.

REFERENCE COUNT: 32 THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

$$\text{O}=\overset{\text{||}}{\text{Cl}}-\text{O}^-$$

CRN 14797-73-0 CMF CL 04

2 CM



PAGE 3-A

**spectrometer.** The complexes of heme and three other metalloporphyrins with a variety of basic **peptides** and model systems were formed via electrospray ionization (ESI) and their stability was probed by energy-variable collision-induced dissociation (CID). A linear dependence for basic **peptides** and model compds./metalloporphyrin was used to evaluate relative bond strength. These results were then compared with previous data obtained for complexes of metalloporphyrins with His-containing **peptides** and **peptides** containing no basic amino acids. The binding strengths of Lys-containing **peptide** complexes in the gas phase is almost as strong as that of Arg-containing complexes. Both systems showed stronger binding than His-containing **peptides** studied previously. To probe the structure of Arg and Lys noncovalent complexes (charge solvation vs. salt bridges), two techniques, CID and ion-mol. reactions, were used. CID expts. indicate that the gas-phase complexes are most likely formed by charge solvation of the central metal ion in the metalloporphyrin by basic side chains of Arg or Lys. Results from the ion-mol. reaction studies are consistent with the charge solvation structure as well.

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 34, 73

ST metalloporphyrin basic **peptide** formation stability structure

**mass spectrometry**; charge solvation structure

metalloporphyrin basic **peptide**; zwitterionic structure

metalloporphyrin basic **peptide**

IT **Peptides**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(basic; stability and structure of metalloporphyrin complexes with basic **peptides** studied by **mass spectrometry**)

)

IT Molecular structure

(of metalloporphyrin complexes with basic **peptides** studied by **mass spectrometry**)

IT Transition metal complexes

RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(porphyrin; stability and structure of metalloporphyrin complexes with basic **peptides** studied by **mass spectrometry**)

)

IT Collision-induced dissociation

Ion-molecule reaction

Mass spectra

(stability and structure of metalloporphyrin complexes with basic **peptides** studied by **mass spectrometry**)

IT Metalloporphyrins

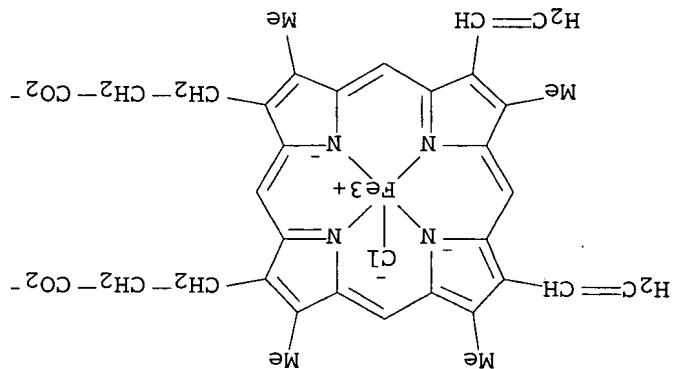
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)

(transition metal; stability and structure of metalloporphyrin complexes with basic **peptides** studied by **mass spectrometry**)

IT 56-87-1D, L-Lysine, metalloporphyrin complexes 74-79-3D, L-Arginine, metalloporphyrin complexes 107-43-7D, Betaine, metalloporphyrin complexes 541-15-1D, L-Carnitine, metalloporphyrin complexes 687-64-9D, L-Lysine methyl ester, metalloporphyrin complexes 997-62-6D, metalloporphyrin complexes 2577-94-8D, metalloporphyrin complexes 6249-56-5D, 3-Carboxypropyltrimethylammonium chloride, metalloporphyrin complexes 15958-92-6D, 1-8-Bradykinin, metalloporphyrin complexes 16009-13-5D, Hemin chloride, complexes with **peptides** and analogs 16456-81-8D, complexes with **peptides** and analogs

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS PAPER. ALL CITATIONS AVAILABLE IN THE PDF FORMAT

● 2 H<sup>+</sup>



FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

| PATENT NO.    | KIND  | DATE     | APPLICATION NO. | DATE     |
|---------------|-------|----------|-----------------|----------|
| -----         | ----- | -----    | -----           | -----    |
| JP 2004045292 | A1    | 20040212 | JP 2002-204864  | 20020712 |
| US 2004029181 | A1    | 20040212 | US 2003-614324  | 20030708 |

## PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 140:177881

AB A novel metal complex is provided, which is useful as a protein or **peptide** amino acid sequence determination reagent. Also provided is a protein/**peptide** amino acid sequence determination method using the novel metal complex. This metal complex possesses a functional group capable of forming a covalent bond with an amino group of the N-terminal amino acid residue of a protein or **peptide**, or with a carboxyl group of the C-terminal amino acid residue of a protein or **peptide**. Normally, the functional group is contained in a ligand. The method comprises reacting the metal complex with a protein or **peptide** (A) to be analyzed concerning its amino acid sequence, obtaining a metal complex derivative (B) in which a covalent bond is formed between the functional group of the metal complex and the amino group of the N-terminal amino acid residue of the a protein or **peptide**, or the carboxyl group of the C-terminal amino acid residue of the protein or **peptide**, and analyzing the metal complex derivative by a **mass spectrometry** to determine the amino acid sequence of the protein or **peptide**.

IC ICM G01N033-68  
ICS C07D213-22; C07D213-53; C07D213-55; C07D249-18; G01N027-62;  
C07K001-22

CC 9-16 (Biochemical Methods)

ST metal complex protein **peptide** sequence **mass spectrometry**

IT Amino group

Carboxyl group

Coordination number

Functional groups

**Mass spectrometry**

Protein sequences

(novel metal complex, and use in protein sequence determination method)

IT **Peptides**, biological studies

Proteins

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(novel metal complex, and use in protein sequence determination method)

IT Ligands

Reagents

**Transition metals**, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(novel metal complex, and use in protein sequence determination method)

IT 657409-70-6P 657409-72-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(novel metal complex, and use in protein sequence determination method)

IT 657409-70-6P 657409-72-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

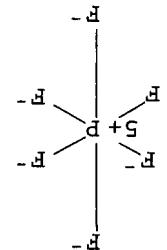
(novel metal complex, and use in protein sequence determination method)

RN 657409-70-6 HCPLUS

CN Ruthenium(1+), (2,2':6',2'''-terpyridine- $\kappa$ N1, $\kappa$ N1', $\kappa$ N1'')[

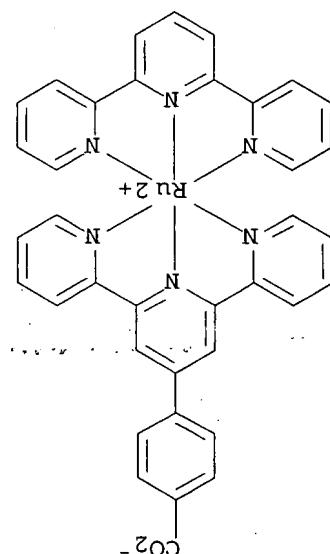
CM 1

(9CI) (CA INDEX NAME)  
 1-[4-([2,2':6,2''-terpyridin]-4-yl-KN<sub>1</sub>,KN<sub>1</sub>,KN<sub>1</sub>)-benzoxy]-2,5-pyrrolidinedione], (OC-6-23)-, bis[hexafluorophosphate(1-)]  
 Ruthenium(2+), (2,2':6,2''-terpyridine-KN<sub>1</sub>,KN<sub>1</sub>,KN<sub>1</sub>)[  
 657409-72-8 HCAPLUS  
 CN



CCl CCS  
 CMF F<sub>6</sub>P  
 CRN 16919-18-9

CM 2



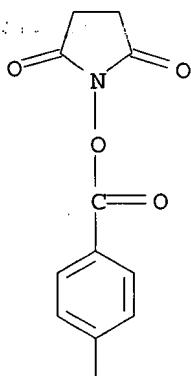
CCl CCS  
 CMF C37 H25 N6 O2 Ru  
 CRN 657409-69-3

CM 1

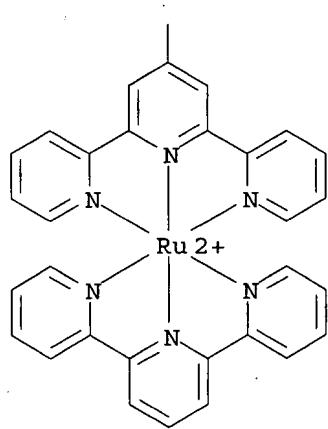
NAME)  
 4-([2,2':6,2''-terpyridin]-4-yl-KN<sub>1</sub>,KN<sub>1</sub>,KN<sub>1</sub>)benzoate  
 O]-, (OC-6-23)-, hydrogen hexafluorophosphate(1-)(1:1:2) (9CI) (CA INDEX

CRN 657409-71-7  
CMF C41 H29 N7 O4 Ru  
CCI CCS

PAGE 1-A



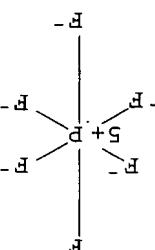
PAGE 2-A



CM 2

CRN 16919-18-9  
CMF F6 P

| AUTHOR(S):         | Sevillano, Paloma; Habtemariam, Abraha; Sejjo, M.; Ines Garciá; Castineiras, Alfonso; Parsons, Simon; García, M. Esther; Sádler, Peter J.  |
|--------------------|--|
| CORPORATE SOURCE:  | Departamento de Química Inorganica, Universidad de Santiago de Compostela, 15706, Spain  |
| SOURCE:            | Australian Journal of Chemistry (2000), 53(8), 635-644 CODEN: AJCHAS; ISSN: 0004-9425  |
| PUBLISHER:         | CSIRO Publishing   |
| DOCUMENT TYPE:     | AB Comp lexes Pd(tripod)X2 [X = Me(CH <sub>2</sub> Ph) <sub>2</sub> ] <sup>3-</sup> ; X = Cl <sup>-</sup> , Br <sup>-</sup> , I <sup>-</sup> ] and Pt(tripod)X2 [X = Cl <sup>-</sup> , Br <sup>-</sup> , I <sup>-</sup> ] were synthesized. In these complexes tripod acts as a bidentate chelating ligand. The uncoordinated P atom can bind to AuI to form the bimetallic complexes PdAu(tripod)X <sub>3</sub> <sup>+</sup> = Cl <sup>-</sup> (7), Br <sup>-</sup> (8), I <sup>-</sup> (9)] and PtAu(tripod)X <sub>3</sub> <sup>+</sup> [X = Cl <sup>-</sup> (10), Br <sup>-</sup> (11), I <sup>-</sup> (12)]. Comp lexes 1-12 were characterized by microanal., FAB mass spectrometry, IR spectroscopy, 31P and 195Pt NMR spectroscopies, and conductivity measurements. The structures of complexes 1-Me <sub>2</sub> CO, 4 and 11, as well as that of the unusual complex Cl <sub>2</sub> Pt(tripod)AuBr <sub>2</sub> ·5ClO <sub>4</sub> (13), isolated from reaction of Pt(tripod)Br <sub>2</sub> (5), and [Au(ethiodiglycol)Cl] <sup>+</sup> were determined. All comp lexes show square planar geometry for PtII and linear geometry for AuI. The x-ray crystal structure for PdII or PtII and oxidation of the dangle ring P of the ligand in 50% of the mol. distributed randomly over the lattice. Reactions of complex 4 with the radical methyl methionine (ACMet) or GMP (5'-GMP) was observed. Reactions of Pd <sup>2+</sup> (tripod)2 (GS- <sup>11</sup> -S) <sub>2</sub> <sup>2+</sup> (14) with GSH gave [Pd <sup>2+</sup> (tripod-O) <sub>2</sub> (GS- <sup>11</sup> -S) <sub>2</sub> <sup>2+</sup> ] (15a). No reaction with N-acetyl-L- <sup>14</sup> S-GMP in the presence of AuI, via P-S bond cleavage, was observed for 15b. PdAu(tripod)Cl <sub>3</sub> 10 (15b). Displacement of the S-containing mol s. by 5'-GMP in the presence of reagents with GSH, with initial attack on the AuI center. |
| ACCESSTION NUMBER: | 2000:901614 HCAPLUS  |
| TITLE:             | Homonuclear PdII and PtII and heteronuclear PdII-AuI and PtII-AuI comp lexes of a tripod trisphosphite.  |
| DOCUMENT NUMBER:   | 134:202146   |
| ACCESSION NUMBER:  | 74 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN   |



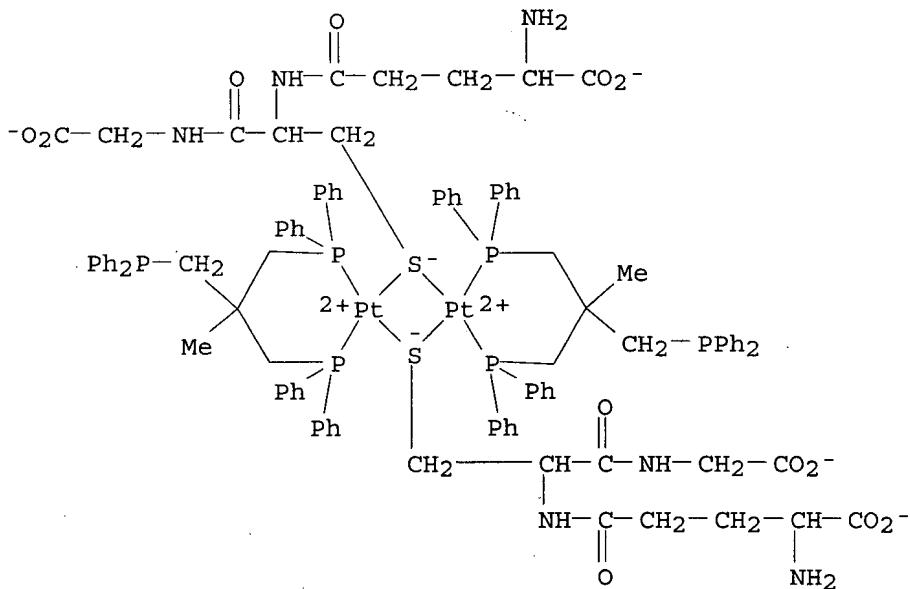
CCS CCI

structure reaction gold; platinum trisdiphenylphosphinoethane prepn  
 reaction gold biomol; phosphinoethane tripodal **transition metal** homonuclear heteronuclear prepn; gold heteronuclear palladium platinum trisdiphenylphosphinoethane prepn; glutathione reaction platinum trisdiphenylphosphinoethane; guanosine monophosphate reaction platinum trisdiphenylphosphinoethane; acetylmetionine reaction platinum trisdiphenylphosphinoethane

IT 327033-73-8 327033-76-1 327033-79-4  
 327033-79-4D, reaction products with 5'GMP in the presence of gold  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation and NMR of)  
 IT 327033-73-8 327033-76-1 327033-79-4  
 327033-79-4D, reaction products with 5'GMP in the presence of gold  
 RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)

(formation and NMR of)  
 RN 327033-73-8 HCPLUS  
 CN Platinato(2-), bis[[2-[(diphenylphosphino)methyl]-2-methyl-1,3-propanediyl]bis[diphenylphosphine- $\kappa$ P]]bis[ $\mu$ -[L- $\gamma$ -glutamyl-L-cysteinyl- $\kappa$ S: $\kappa$ S-glycinato(3-)]di- (9CI) (CA INDEX NAME)

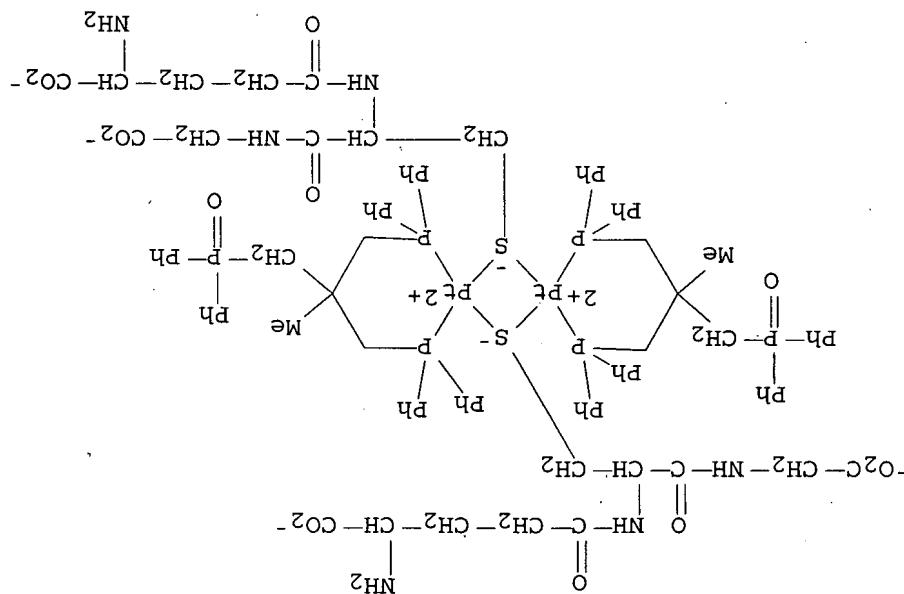


RN 327033-76-1 HCPLUS  
 CN Platinato(2-), dichloro[ $\mu$ -[[2-[(diphenylphosphino- $\kappa$ P)methyl]-2-methyl-1,3-propanediyl]bis[diphenylphosphine- $\kappa$ P]]][[L- $\gamma$ -glutamyl-L-cysteinyl- $\kappa$ S-glycinato(3-)]aurate]-, dihydrogen (9CI) (CA INDEX NAME)

RN 327033-79-4 HCAPLUUS  
 CN  
 PLatinate (2-), bis[[3-(diphenylphosphino)-2-[(diphenylphosphino)-  
 KP)methyl]-2-methyldiropylyl]diphenylphosphine oxide]bis[L-L-]  
 y-glutamyl-L-glycinate (3-)]di-, tetrahydroxogen (9CI) (CA INDEX  
 NAME)

● 4 H+

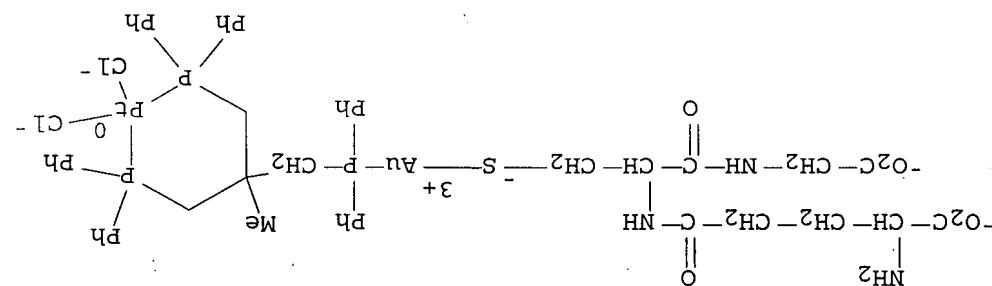
PAGE 2-A



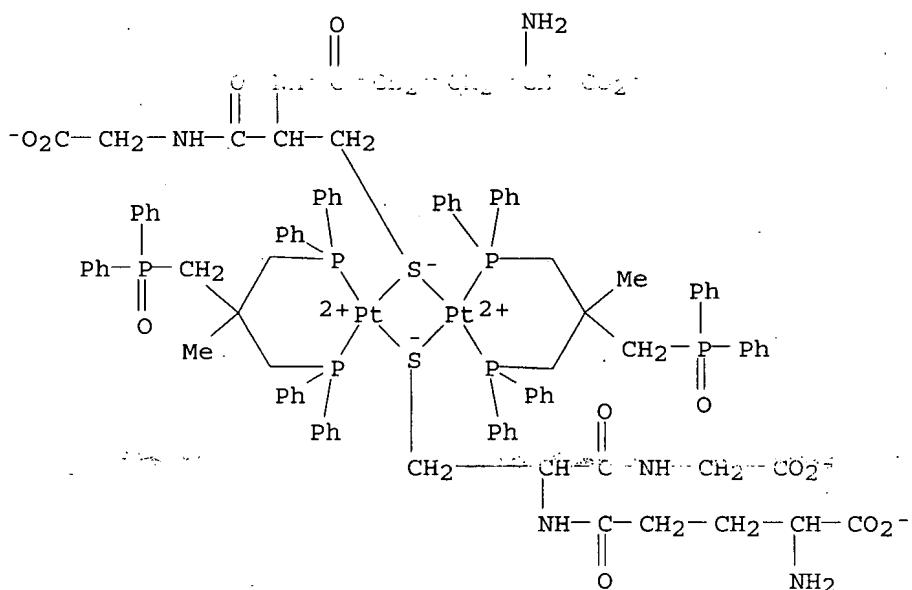
PAGE 1-A

RN 327033-79-4 HCAPLUUS  
 CN  
 PLatinate (2-), bis[[3-(diphenylphosphino)-2-[(diphenylphosphino)-  
 KP)methyl]-2-methyldiropylyl]diphenylphosphine oxide]bis[L-L-]  
 y-glutamyl-L-glycinate (3-)]di-, tetrahydroxogen (9CI) (CA INDEX  
 NAME)

● 2 H+



PAGE 1-A



PAGE 2-A

● 4 H<sup>+</sup>

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 8 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:836623 HCPLUS

DOCUMENT NUMBER: 134:193701

TITLE: Compositions and conformations of several transition metal complexes with a nonapeptide hormone oxytocin

AUTHOR(S): Wei, Hua; Luo, Xuemei; Wu, Yibing; Yao, Yong; Guo, Zijian; Zhu, Longgen

CORPORATE SOURCE: Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry, Nanjing University, Nanjing, 210093, Peop. Rep. China

SOURCE: Dalton (2000), (22), 4196-4200  
CODEN: DALTFG

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Similar co-ordination characteristics of oxytocin (OT) towards CuII, NiII, MnII and ZnII at different pH values have been demonstrated by electrospray mass spectrometry (ESMS) and rationalized by mol. mechanics simulation. At ca. pH 2 oxytocin does not interact with the metal ions; at pH 5 species with metal bound oxytocin were detected, including [OT + H+]<sup>+</sup>, [M + OT]<sup>2+</sup>, [M + OT - H+]<sup>+</sup>, [M + OT + ClO<sub>4</sub><sup>-</sup> + H+]<sup>2+</sup> and [M + OT + ClO<sub>4</sub><sup>-</sup>]<sup>+</sup> and only stable 4N complexes were found at pH ≈ 9. Mol. modeling studies using the Universal force field (UFF) showed that the four N-donor centers of oxytocin prefer the square planar

geometry in complexes of NiII and MnII. For PdII, the S<sub>γ</sub>(1) coordinated conformer was found to be more stable than the S<sub>γ</sub>(6) coordinated one. Dramatic conformational changes occur upon oxytocin co-ordinating to NiII, MnII or PdII.

CC 34-3 (Amino Acids, Peptides, and Proteins)  
Section cross-reference(s): 2, 78

ST oxytocin complex **transition metal** conformation ESMS  
mol mechanics simulation; conformation complex **transition metal** oxytocin mol modeling

IT Conformation  
Electrospray ionization **mass spectrometry**  
Molecular mechanics  
Molecular modeling  
Simulation and Modeling, physicochemical  
(conformations of **transition metal** complexes with  
oxytocin)

IT **Transition metal complexes**  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(conformations of **transition metal** complexes with  
oxytocin)

IT 328123-81-5  
RL: PRP (Properties)  
(conformations of **transition metal** complexes with  
oxytocin)

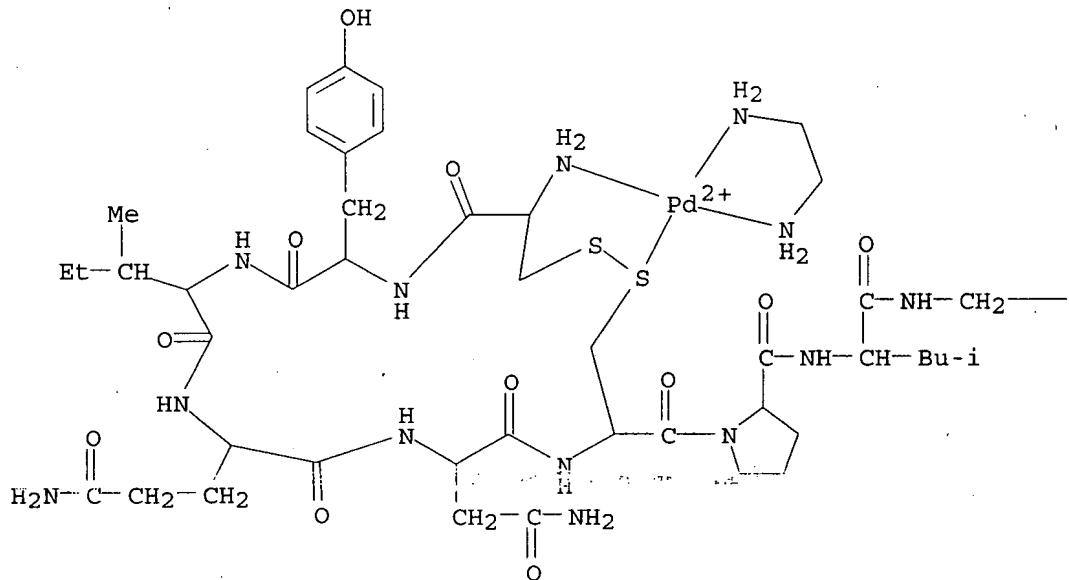
IT 50-56-6DP, Oxytocin, **transition metal complexes**,  
preparation 50-56-6P, Oxytocin, preparation 7439-96-5DP, Manganese,  
oxytocin complexes, preparation 7440-02-0DP, Nickel, oxytocin complexes,  
preparation 7440-50-8DP, Copper, oxytocin complexes, preparation  
7440-66-6DP, Zinc, oxytocin complexes, preparation 222716-70-3P  
328123-77-9P 328123-78-0P 328123-79-1P  
328123-80-4P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(conformations of **transition metal** complexes with  
oxytocin)

IT 328123-81-5  
RL: PRP (Properties)  
(conformations of **transition metal** complexes with  
oxytocin)

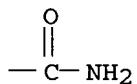
RN 328123-81-5 HCAPLUS

CN Palladium(2+), (oxytocin-κN1,κS)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



IT 222716-70-3P 328123-77-9P 328123-78-0P

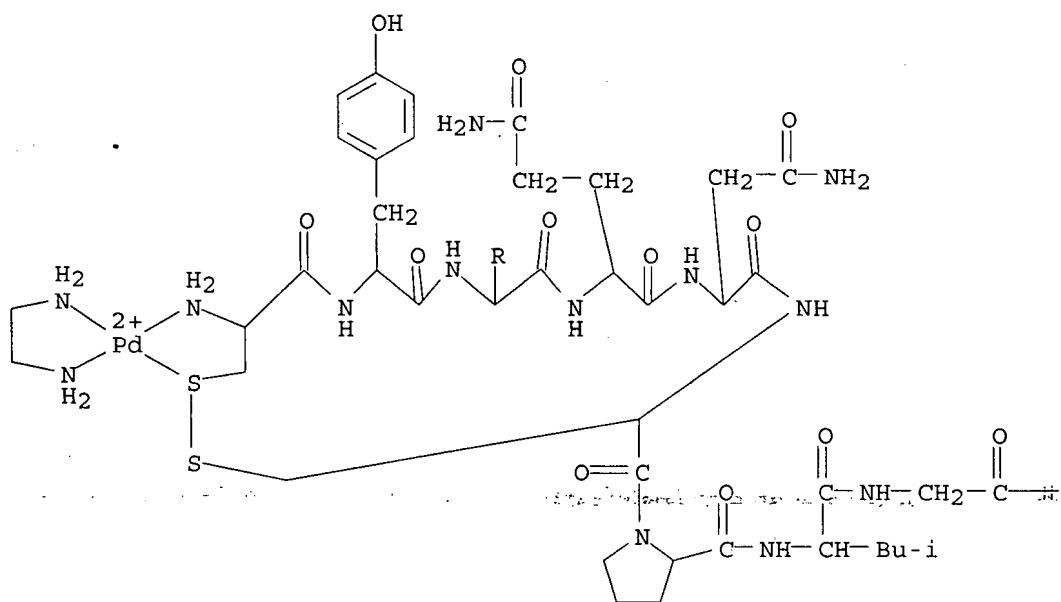
328123-79-1P 328123-80-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(conformations of transition metal complexes with  
oxytocin)

RN 222716-70-3 HCPLUS

CN Palladium(2+), (1,2-ethanediamine-κN1,κN2) (oxytocin-  
κN1,κS1)-, (SP-4-3)- (9CI) (CA INDEX NAME)

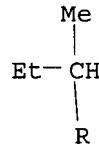
PAGE 1-A



PAGE 1-B

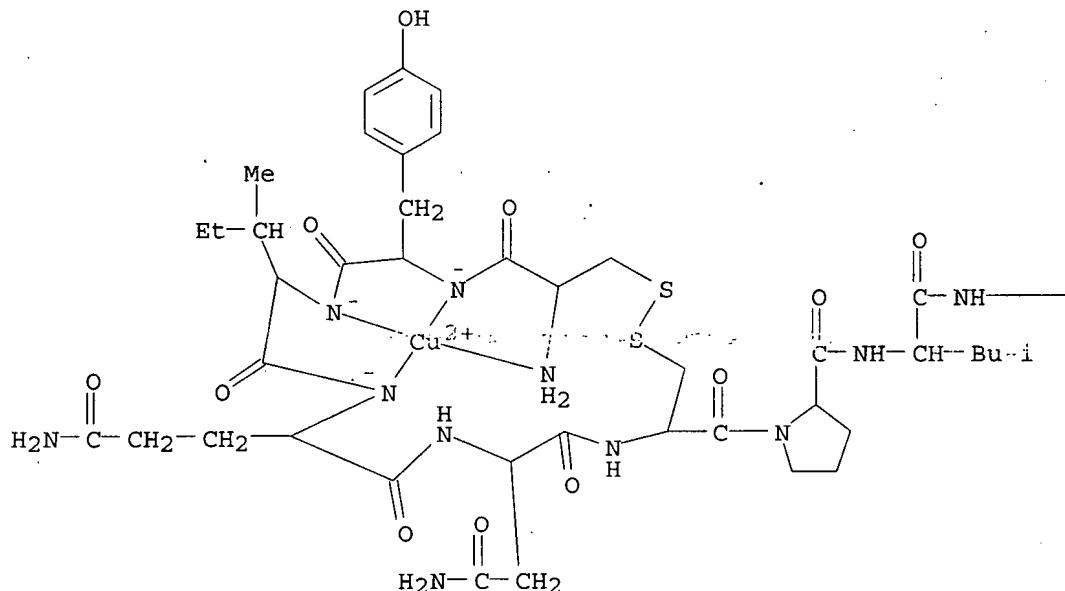
—NH<sub>2</sub>

PAGE 2-A

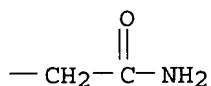


RN 328123-77-9 HCPLUS  
 CN Cupratè(1-) , [oxytocinato(4-) -κN1, κN2, κN3, κN4] -  
 (9CI) (CA INDEX NAME)

PAGE 1-A

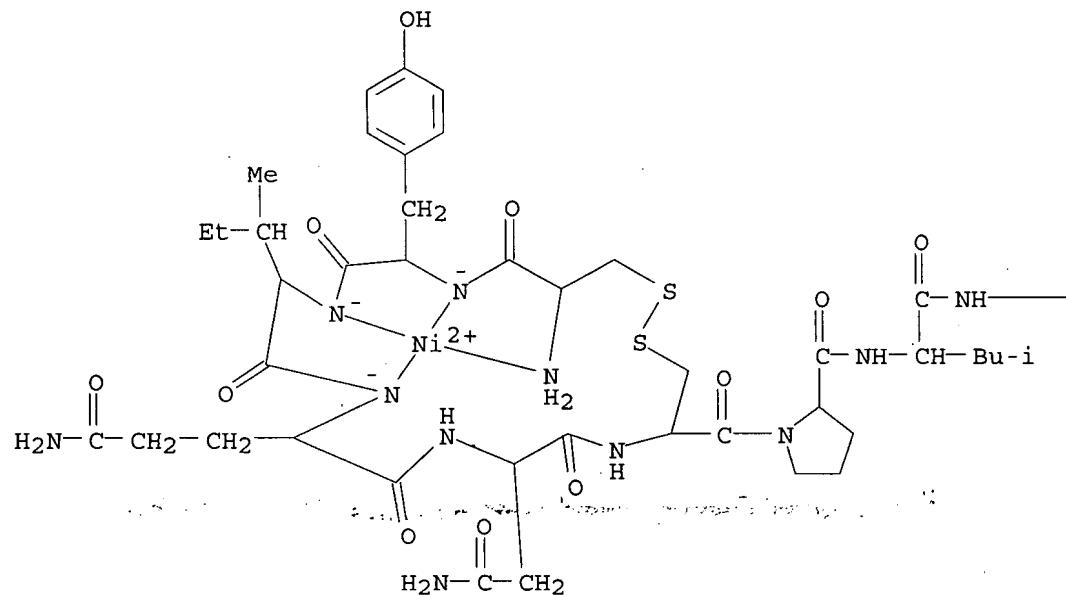


PAGE 1-B

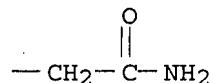


RN 328123-78-0 HCPLUS  
 CN Nickelate(1-) , [oxytocinato(4-) -κN1, κN2, κN3, κN4] -  
 (SP-4-2) - (9CI) (CA INDEX NAME)

PAGE 1-A



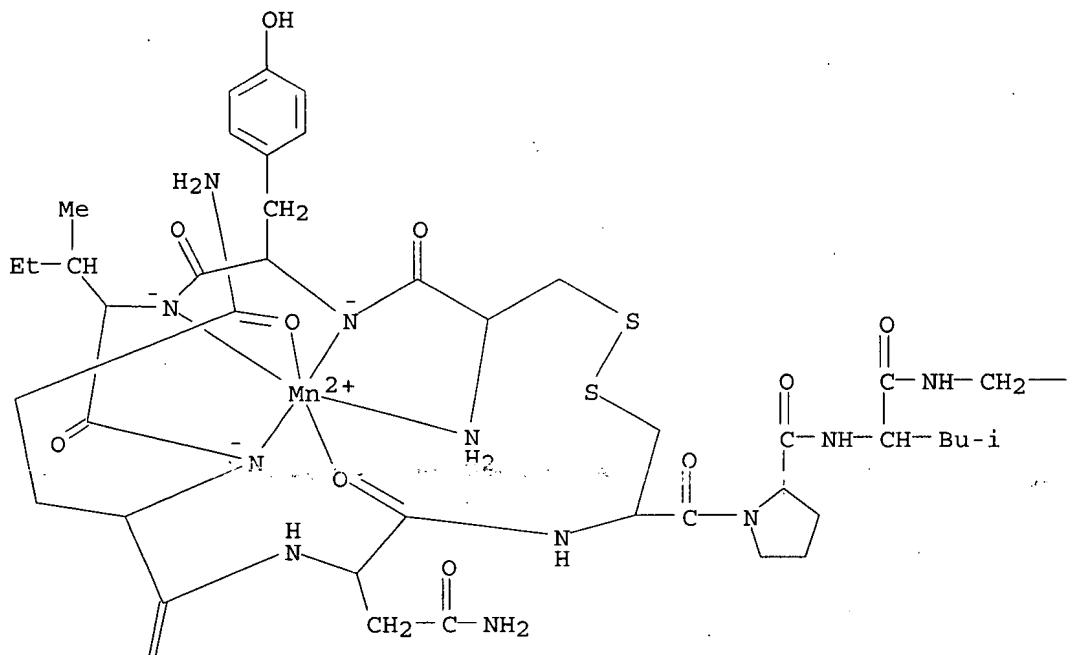
PAGE 1-B



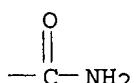
RN 328123-79-1 HCPLUS

CN Manganate(1-), [oxytocinato(3-) - $\kappa$ N1,  $\kappa$ N2,  $\kappa$ N3,  $\kappa$ N4, . k appa.O4,  $\kappa$ O5] - (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

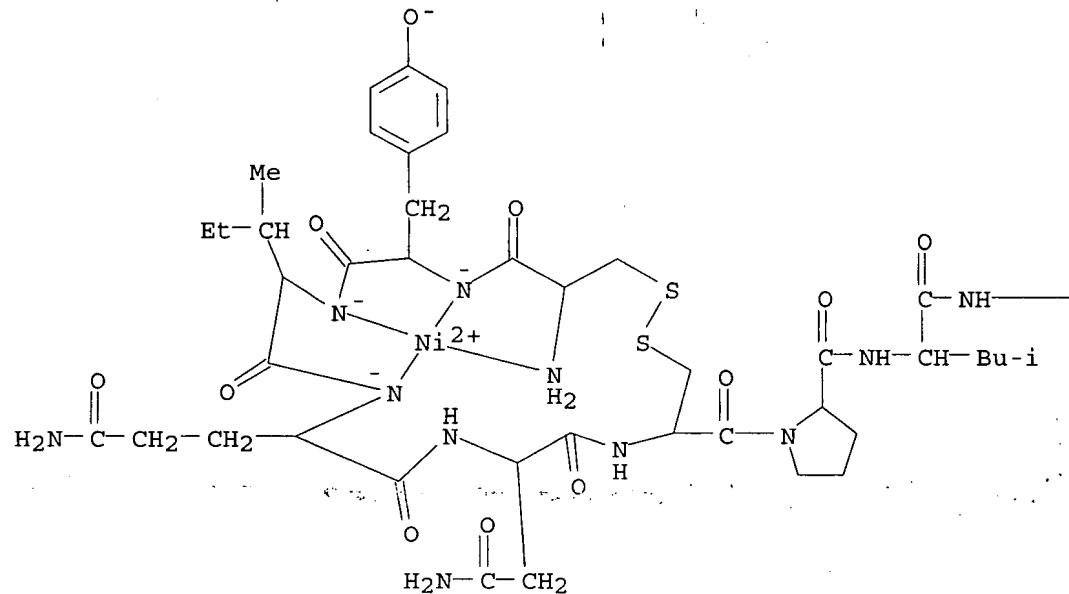


PAGE 2-A

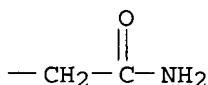
$$\begin{array}{c} // \\ \backslash \end{array}$$

RN 328123-80-4 HCAPLUS  
 CN Nickelate(2-), [oxytocinato(4-) -κN1, κN2, κN3, κN4] -,  
 (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L74 ANSWER 9 OF 9 HCPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1998:764566 HCPLUS

DOCUMENT NUMBER: 130:101169

TITLE: A catalytic activity of glass beads, silica gels and anion-exchange resins modified with metal-porphines in oxidative reactions of ascorbic acid

AUTHOR(S): Iwado, Akimasa; Mifune, Masaki; Harada, Harada; Akizawa, Hiromichi; Motohashi, Noriko; Saito, Yutaka

CORPORATE SOURCE: Graduate School of Natural Science and Technology, Okayama University, Okayama, 700-8530, Japan

SOURCE: Inorganica Chimica Acta (1998), 283(1), 44-50

CODEN: ICHAA3; ISSN: 0020-1693

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB An anion-exchange resin was modified with metal-tetrakis(4-sulfophenyl)porphine (M-TSPP) by ion-exchange reaction and phys. adsorption, and silica gels and glass beads were modified by using the acid chloride of metal-tetrakis(4-carboxyphenyl)porphine (M-TCPP) through the peptide bond. The supports modified with Co<sup>3+</sup>-porphine accelerate the following redox reaction(s), of which the former is also catalyzed by ascorbate-oxidase (AsA): 2(ascorbate (AsA)+) + O<sub>2</sub> ASO<sub>4</sub> or supports modified with M-porphine → 2(dehydroascorbate (DhAsA)) + 2H<sub>2</sub>O; ascorbate (AsA) + O<sub>2</sub> supports modified with M-porphine → dehydroascorbate (DhAsA) + H<sub>2</sub>O<sub>2</sub>. Formation of DhAsA and H<sub>2</sub>O<sub>2</sub> was confirmed by mass spectrometry and colored reaction, resp. The supports modified with Co<sup>3+</sup>-porphine would be useful in practice as solid catalysts for the determination of AsA and for the removal of AsA which interferes with the determination of vital materials in clin. assays.

CC 67-1 (Catalysis, Reaction Kinetics, and Inorganic Reaction Mechanisms)

ST Section cross-reference(s): 34

oxidn catalyst transition metal porphine supported ascorbic acid; glass bead support transition metal porphine oxidn catalyst; silica gel support transition metal porphine oxidn catalyst; anion exchange reaction support transition metal porphine oxidn catalyst

IT Glass beads

Silica gel, uses

RL: NUU (Other use, unclassified); USES (Uses)  
 (support for transition metal porphines as oxidation catalysts for ascorbic acid)

IT Oxidation catalysts

(transition metal porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)

IT 9050-97-9, Amberlite IRA 900 53025-53-9, Dowex MSC-1

RL: NUU (Other use, unclassified); USES (Uses)  
 (support for transition metal porphines as oxidation catalysts for ascorbic acid)

IT 39174-47-5 51329-41-0 60489-11-4 80004-36-0 87261-81-2  
 88992-32-9 91629-46-8 95763-38-5 129102-32-5 137090-57-4  
 211232-23-4

RL: CAT (Catalyst use); USES (Uses)  
 (transition metal porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)

IT 50-81-7, Ascorbic acid, reactions

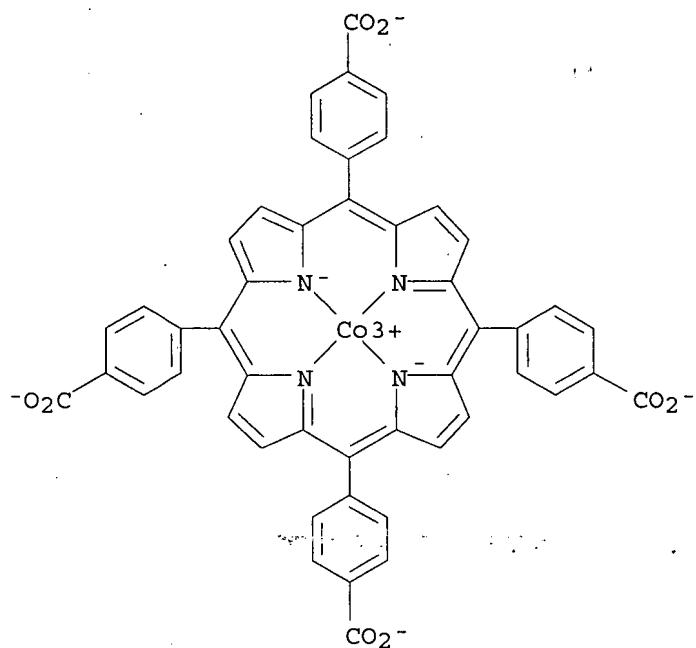
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (transition metal porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)

IT 137090-57-4

RL: CAT (Catalyst use); USES (Uses)  
 (transition metal porphines supported on glass beads, silica gels and anion-exchange resins as oxidation catalysts for ascorbic acid)

RN 137090-57-4 HCPLUS

CN Cobaltate(3-), [[4,4',4'',4'''-(21H,23H-porphine-5,10,15,20-tetrayl)tetrakis[benzoato]](6-)·κN21,κN22,κN23,κN24]-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

16

THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT